CS598PS Machine Learning for Signal Processing

Features Part II – ICA and NMF

11 September 2015

UNIVERSITY OF ILLINOIS AT URBANA-CHAMPAIGN

Today's lecture

- What comes after PCA
- Independent Component Analysis
  - Achieving complete "decorrelation"
- Non-Negative Matrix Factorization

PCA and decorrelation

- Goal of PCA
  - Diagonalize the covariance

$$\mathbf{x}^\top \cdot \mathbf{y} = E\{xy\} = 0$$

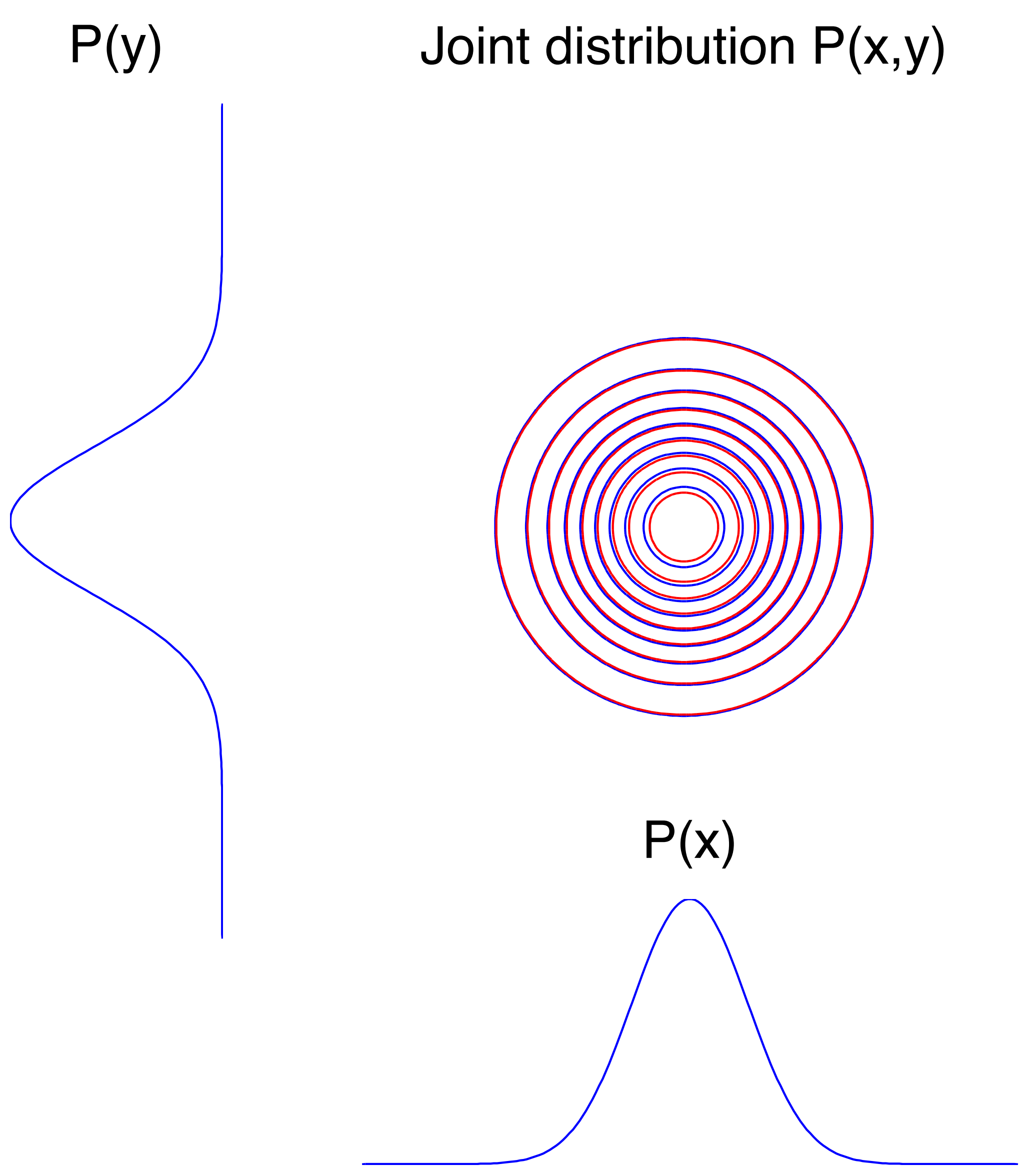
    - i.e. Decorrelate the feature weights
- Why?
  - We want to have the features activated in a statistically independent manner
    - So that they capture more structure

Statistical Independence

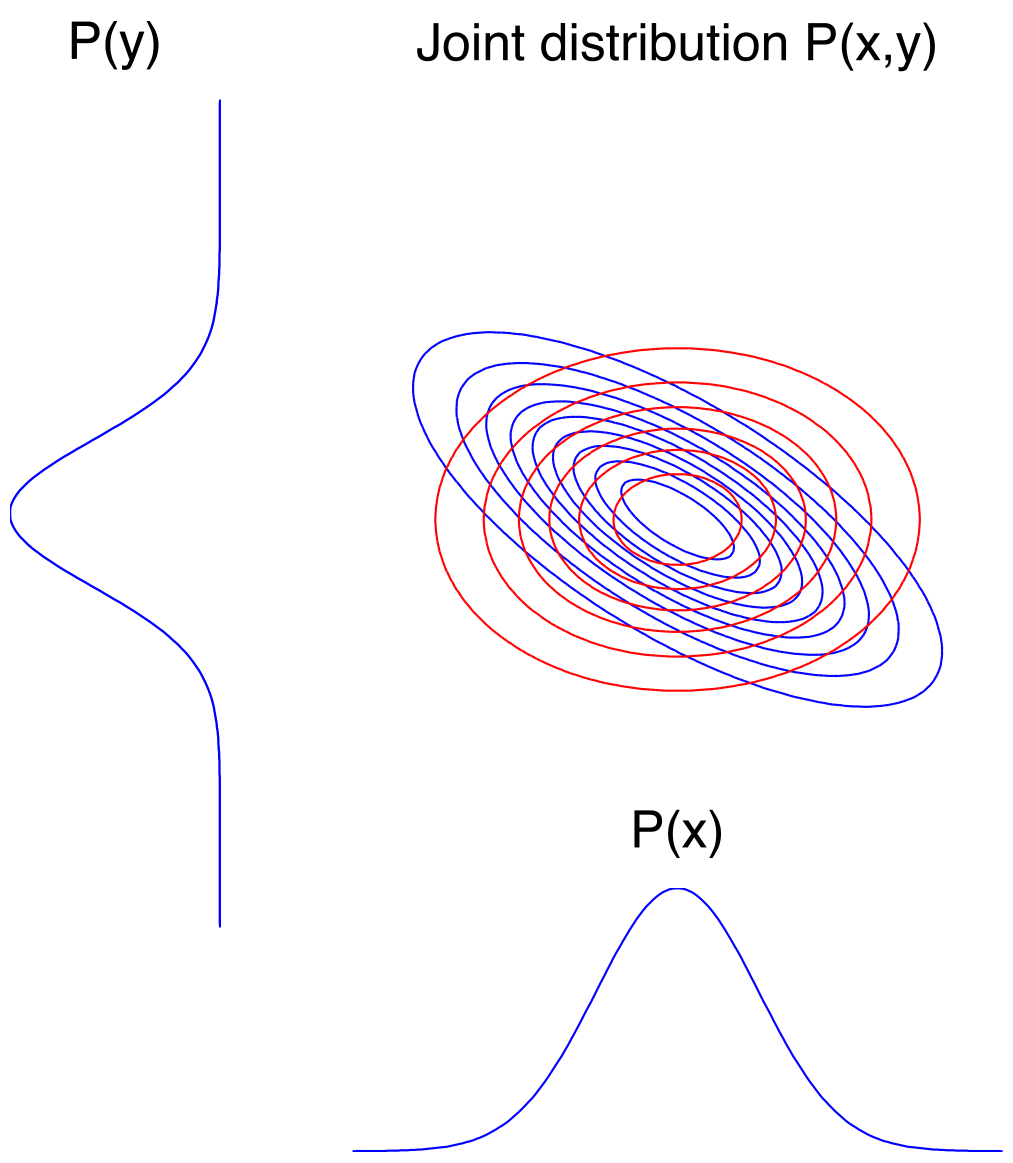
- We defined statistical independence as:

$$P(x,y) = P(x)P(y)$$

Independent variables



Dependent variables



Statistical Independence

- We defined statistical independence as:

$$P(x,y) = P(x)P(y)$$

- Which implies:

$$E\{f(x)g(y)\} = E\{f(x)\}E\{g(y)\}$$

  - For all measurable functions f and g
- Essentially independence means that we can't tell anything about x if we observe y

Decorrelation and Independence

- Decorrelation does not imply independence!
  - Decorrelation: $E\{xy\} = E\{x\}E\{y\}$
  - Independence: $E\{f(x)g(y)\} = E\{f(x)\}\{g(y)\}$
- But independence implies decorrelation
  - When f and g are identity functions
  - Independence is a superset of decorrelation

Decorrelation and Independence

- An example with discrete variables
  - Are they uncorrelated?

	$x == -1$	$x == 0$	$x == 1$
$y == -1$	0	$^1/_4$	0
$y == 0$	$^1/_4$	0	$^1/_4$
$y == 1$	0	$^1/_4$	0

Decorrelation and Independence

- An example with discrete variables
  - Are they correlated?

	$x == -1$	$x == 0$	$x == 1$
$y == -1$	0	$^1/_4$	0
$y == 0$	$^1/_4$	0	$^1/_4$
$y == 1$	0	$^1/_4$	0

  - x,y are uncorrelated

$$E\{xy\} = E\{x\}E\{y\} = 0$$

Decorrelation and Independence

- An example with discrete variables
  - Are they independent?

	$x == -1$	$x == 0$	$x == 1$
$y == -1$	0	$^1/_4$	0
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Decorrelation and Independence

- An example with discrete variables
  - Are they independent?

	$x == -1$	$x == 0$	$x == 1$
$y == -1$	0	$1/4$	0
$y == 0$	$1/4$	0	$1/4$
$y == 1$	0	$1/4$	0

- x,y are not statistically independent

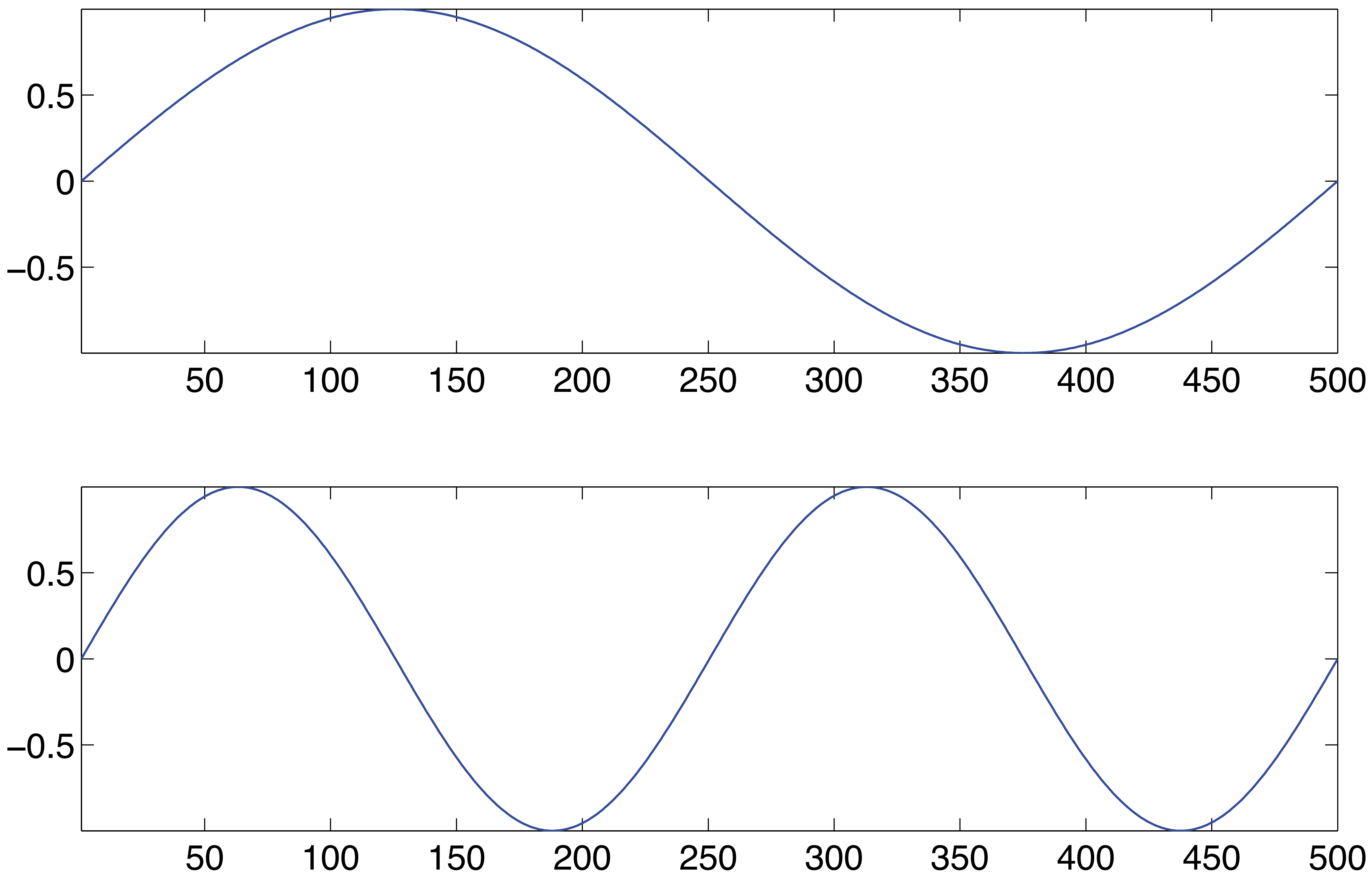
$$E\{x^2y^2\} = 0 \neq E\{x^2\}E\{y^2\} = \tfrac{1}{4}$$

The signals version

- Decorrelated?

$$x = \sin(t)$$

$$y = \sin(2t)$$

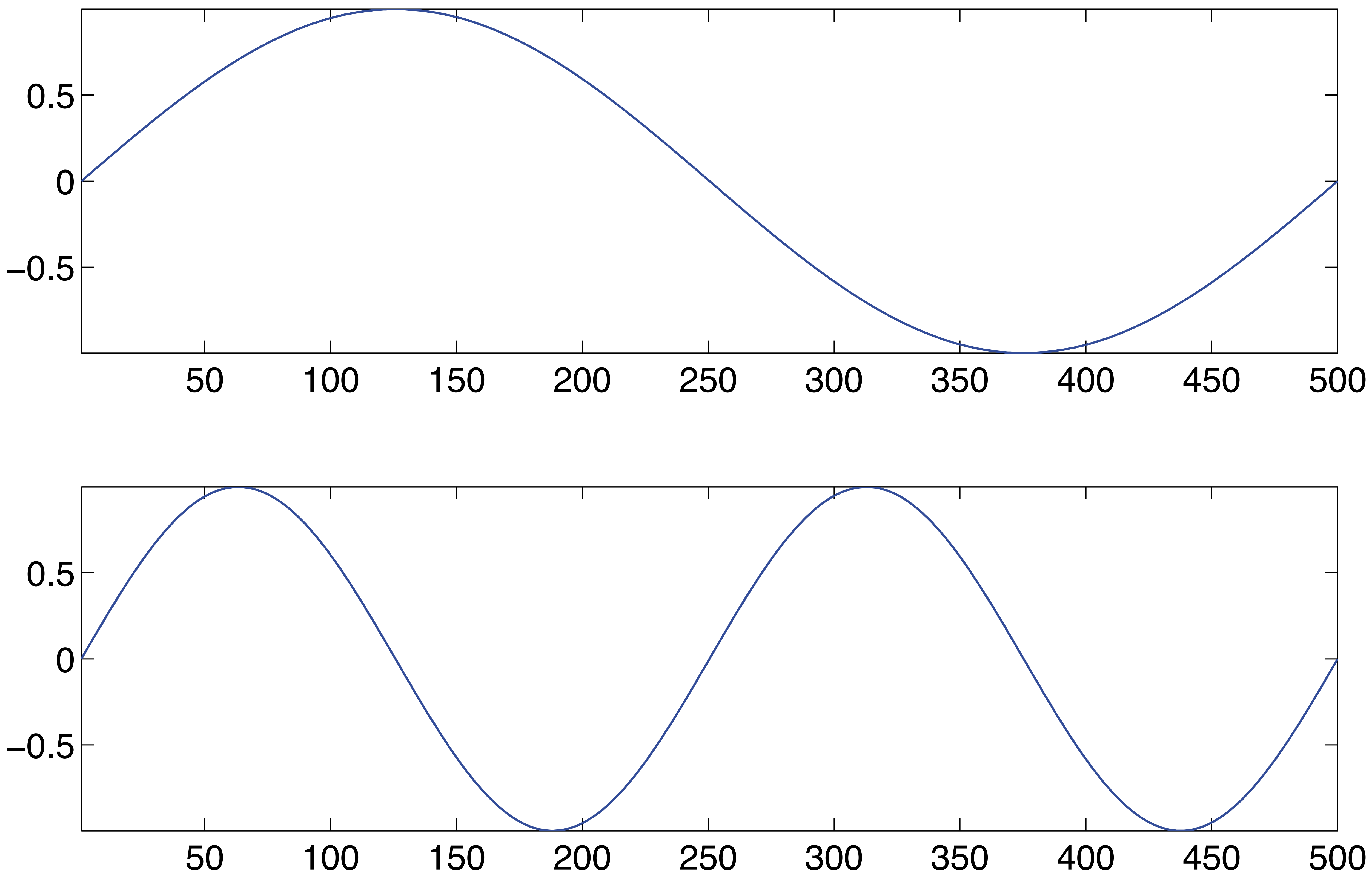


The signals version

- Decorrelated?

$$x = \sin(t)$$
$$y = \sin(2t)$$

- Yes: $E\{xy\} = 0$
  - But I can predict one from the other
  - Not independent!



So how do we get independence?

- Multiple ways of dealing with the problem
  - Family of algorithms known as ICA
    - Independent Component Analysis
- Formal definition:

Analysis Features

Decomposition *Input*

$$\mathbf{y} = \mathbf{W} \cdot \mathbf{x}$$

$$P(y_i, y_j) = P(y_i)P(y_j), \forall i, j$$

Approach 1

- Non-linear decorrelation (assume zero mean inputs from now on)
  - Achieve: $E\{f(y_i)g(y_j)\} = 0$
    - for a fixed f and g
- Cichocki-Unbehauen algorithm
  - Stops updating when independence holds

$$
\begin{aligned}
&\text{do} \\
&\quad \Delta\mathbf{W} \propto \left(\mathbf{D} - f(\mathbf{y}_i)\cdot g(\mathbf{y}_i^\top)\right)\cdot\mathbf{W} \\
&\quad \mathbf{W} = \mathbf{W} + \mu\Delta\mathbf{W} \\
&\text{repeat}
\end{aligned}
$$

$$
\mathbf{D} = \begin{bmatrix} d_1 & & 0 \\ & \ddots & \\ 0 & & d_n \end{bmatrix}
$$

$f(x), g(x)$ can be $\tanh(x), x^3, \ldots$

Approach 2

- Higher-order "diagonalization"
  - In PCA we diagonalized the covariance matrix
    - which is a $N \times N$ structure (a matrix)

$$\mathrm{Cov}(y)_{i,j} = E\{y_i y_j\} = \kappa_2(y_i, y_j)$$

  - In ICA we also diagonalize the quadricovariance tensor
    - which is a $N \times N \times N \times N$ structure (a tensor!)

$$Q(y)_{i,j,k,l} = \kappa_4(y_i, y_j, y_k, y_l) = E\{y_i y_j y_k y_l\} - E\{y_i y_j\}E\{y_k y_l\} - E\{y_i y_k\}E\{y_j y_l\} - E\{y_i y_l\}E\{y_j y_k\}$$

    - confused yet?

Approach 2

- Conceptually we perform a tensor singular value decomposition

- Comon's algorithm
  - 1) Do PCA
    - Imposes decorrelation (halfway there)
  - 2) Find unitary transform that minimizes fourth order cross-cumulants

Approach 3

- Information theoretic optimization
  - Minimize mutual information: $I(\mathbf{y}) = \sum H(y_k) - H(\mathbf{y})$
  - Which implies minimizing: $D(\mathbf{y}) = -\int P(\mathbf{y}) \log \frac{P(\mathbf{y})}{\prod P(y_k)}$
- **Iterative rule:** $\Delta \mathbf{W} \propto (\mathbf{I} - f(\mathbf{y}) \cdot \mathbf{y}^\top) \cdot \mathbf{W}$
  - Looks familiar?

Approaches 4, 5, …

- Maximum likelihood
- FastICA
  - A fast fixed-point algorithm
- Neural nets
  - Directly optimize KL divergence/Mutual information
- Negentropy
  - A measure of non-gaussianity
- …

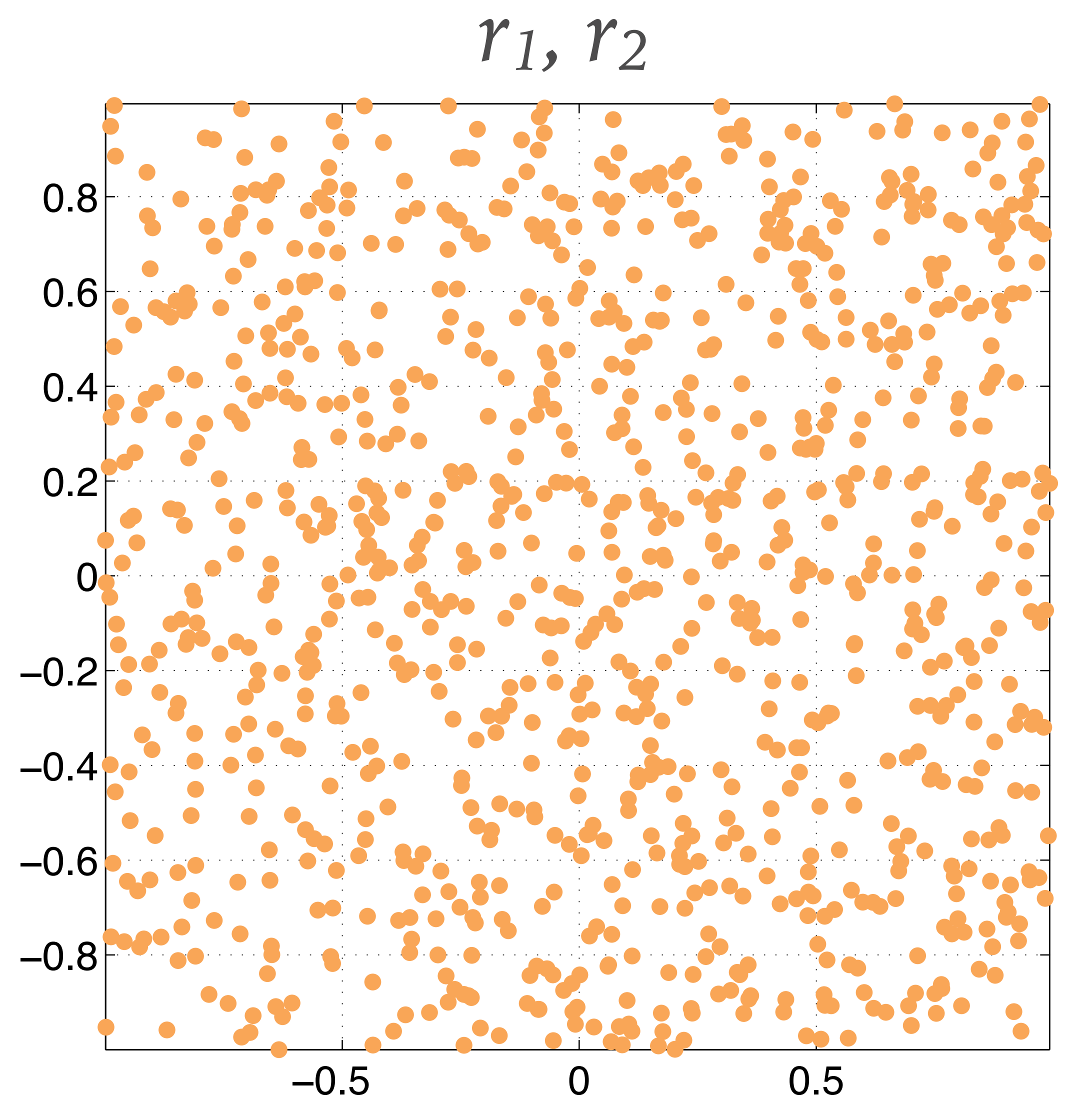
What approach works best?

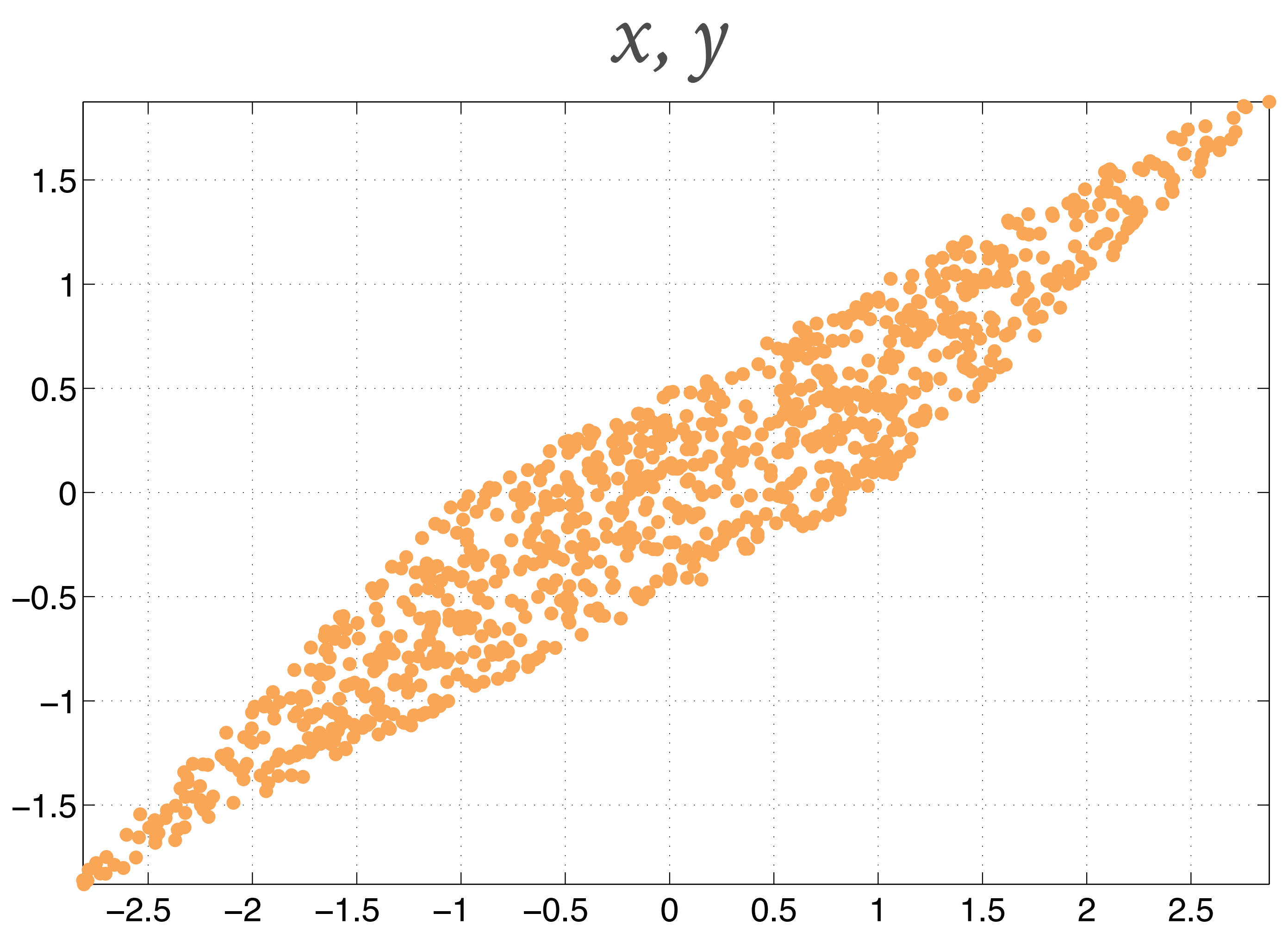
- As usual, no good answer …
- Algebraic algorithms
  - HSVD, cumulant tensors, etc.
  - Computationally demanding
- Iterative algorithms
  - Non-linear decorrelation, infomax, etc
  - Small, fast, but prone to blowups
- FastICA
  - Fixed-point algorithm
  - Quite robust and reliable

So what does ICA do?

- Take two uniform RVs and mix them

$$r_1, r_2 \sim U(-1,1)$$
$$x = 2r_1 + r_2$$
$$y = r_1 + r_2$$

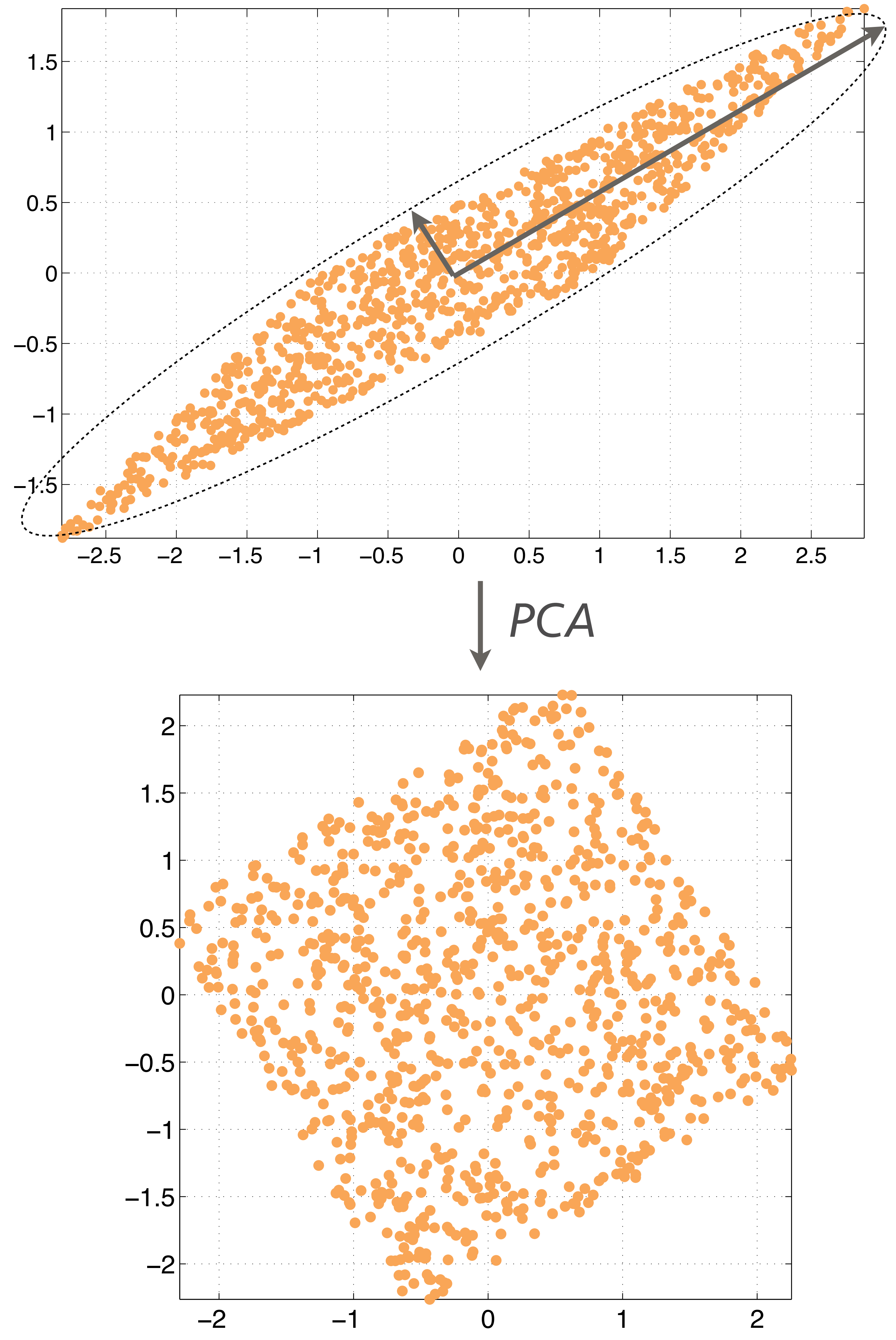




- This creates a dependent x and y
  - Seen as rotation and stretching of data

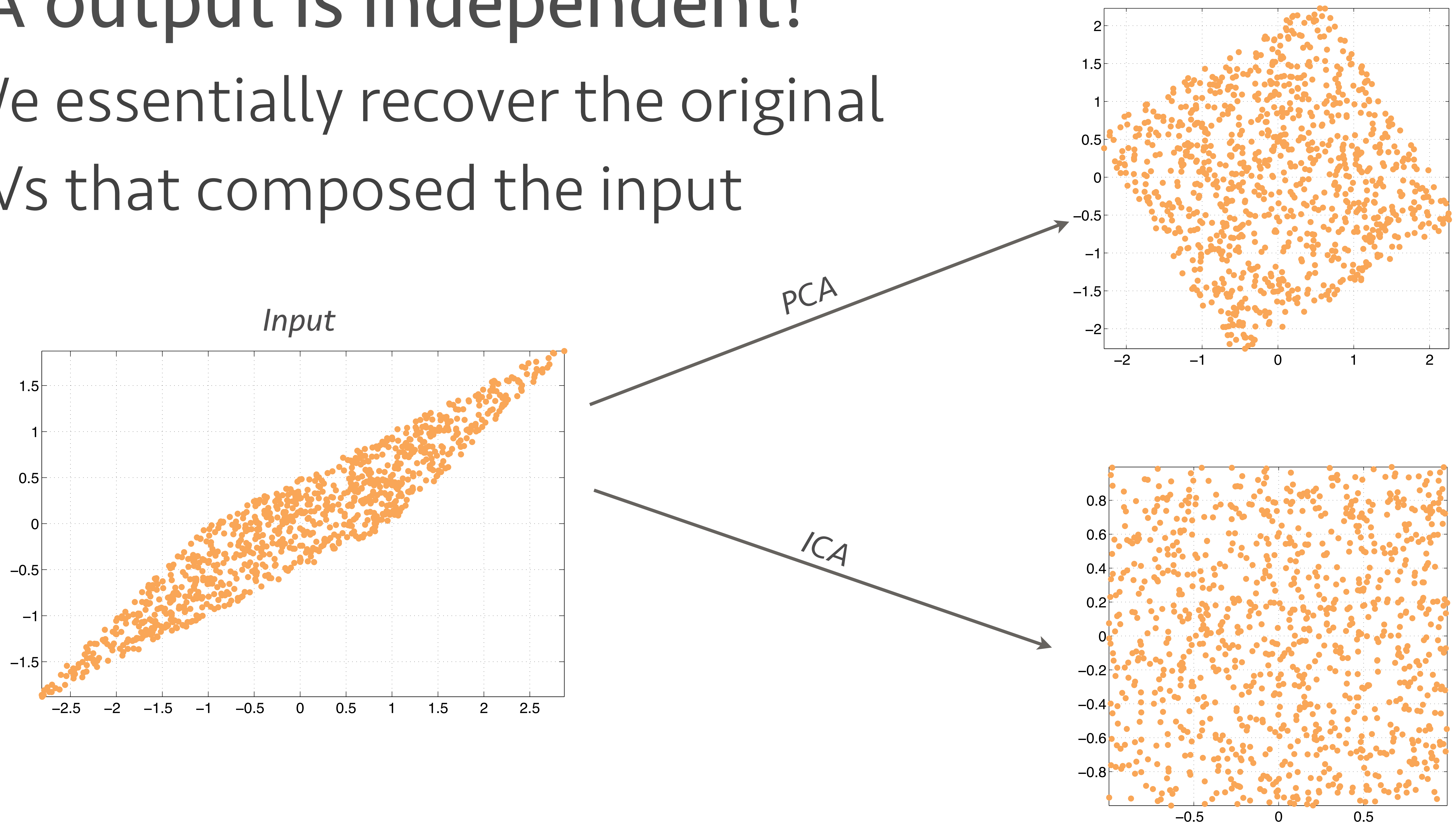
Performing PCA

- PCA will decorrelate
  - Note that rotation highlights maximal variance directions
- The resulting projection has not produced independence



So what does ICA do?

- ICA output is independent!
  - We essentially recover the original RVs that composed the input



ICA issues

- Most estimators are approximate
  - The resulting output is not necessarily the correct one
- There might not be independence
  - ICA returns a <u>maximally independent projection</u>, not an independent one
    - Again the output might not be what you expected to get!

ICA limitations

- Invariance to output permutations

$$P(y_1, y_2, y_3) = P(y_1)P(y_2)P(y_3) = P(y_2)P(y_1)P(y_3) = \ldots$$

  - Output order is not guaranteed and can differ through runs
- No sense of ordering of components
  - PCA orders outputs in terms of variance
  - ICA doesn't have an order
    - As a result we can't reduce dimensionality!

Combining PCA and ICA

- If we need to perform dimensionality reduction we precede ICA with PCA
  - 1) Use PCA to reduce dimensionality
  - 2) Use ICA to impose independence
    - Apply ICA on the output of the PCA
- That's ok, since ICA is a generalization of PCA

So what about the features?

- How do ICA and PCA features differ?
- ICA features provide a more compact/sparse “code”
  - PCA “code” can still have statistical dependencies
- PCA features and projection are decorrelated
  - There is no constraint on the ICA features
  - Only the decomposition output is independent

Analysis vs. synthesis features

- One more distinction to make

- PCA features are "bi-directional"

$$\mathbf{z} = \mathbf{W} \cdot \mathbf{x}$$

$$\hat{\mathbf{x}} = \mathbf{W}^\top \cdot \mathbf{z}$$

- That won't hold anymore
  - We have analysis features: $\mathbf{z} = \mathbf{W} \cdot \mathbf{x}$
  - And synthesis features: $\hat{\mathbf{x}} = \mathbf{W}^+ \cdot \mathbf{z}$

Be careful when combining the two!

- If we want both dimensionality reduction and independence
  - Step 1: Do PCA to reduce the dimensions

$$\mathbf{Z}_P = \mathbf{W}_P \cdot \mathbf{X}, \quad \mathbf{X} \in \mathbb{R}^{M\times N}, \mathbf{W}_P \in \mathbb{R}^{K\times M}, \mathbf{Z}_P \in \mathbb{R}^{K\times N}$$

  - Step 2: Do ICA on the PCA weights to produce independence

$$\mathbf{Z}_I = \mathbf{W}_I \cdot \mathbf{Z}_p, \quad \mathbf{W}_I \in \mathbb{R}^{K\times K}, \mathbf{Z}_I \in \mathbb{R}^{K\times N}$$

- What's what?
  - Analysis features: $\mathbf{Z}_I = \left(\mathbf{W}_I \cdot \mathbf{W}_P\right) \cdot \mathbf{X} \Rightarrow \mathbf{W} = \mathbf{W}_I \cdot \mathbf{W}_P, \quad \mathbf{W} \in \mathbb{R}^{K\times M}$
  - Synthesis features: $\hat{\mathbf{X}} = \left(\mathbf{W}_I \cdot \mathbf{W}_P\right)^{+} \cdot \mathbf{Z}_I$

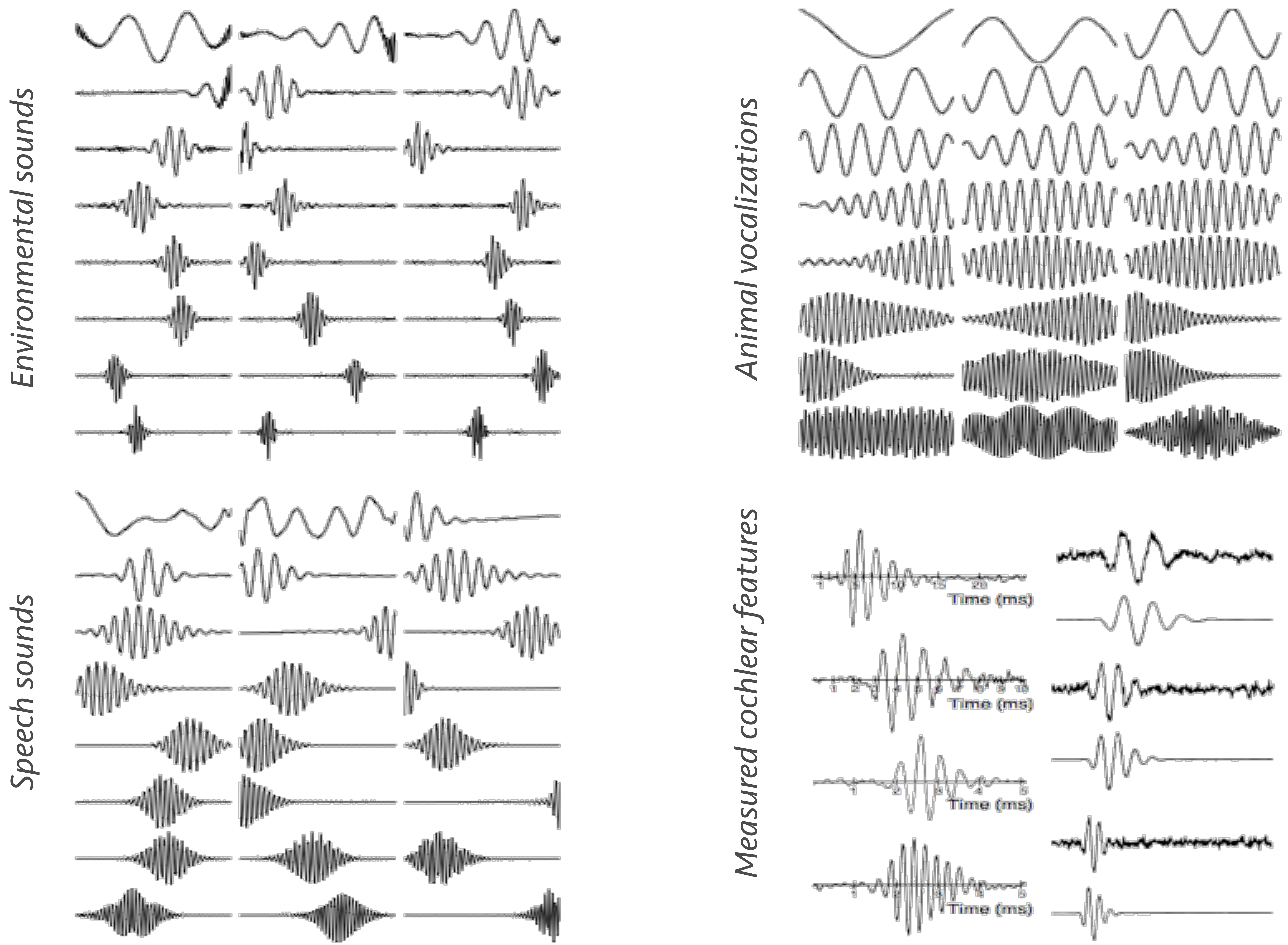
Example features from sounds

- Obtain lots and lots of natural sounds
  - E.g. sounds found in nature, birds, walking on leafs, etc.
- Place short windows in a large matrix
  - and do PCA and ICA

$$\mathbf{Z} = \mathbf{W} \cdot \begin{bmatrix} x(t) & x(t+1) & \\ \vdots & \vdots & \cdots \\ x(t+N) & x(t+1+N) & \end{bmatrix}$$

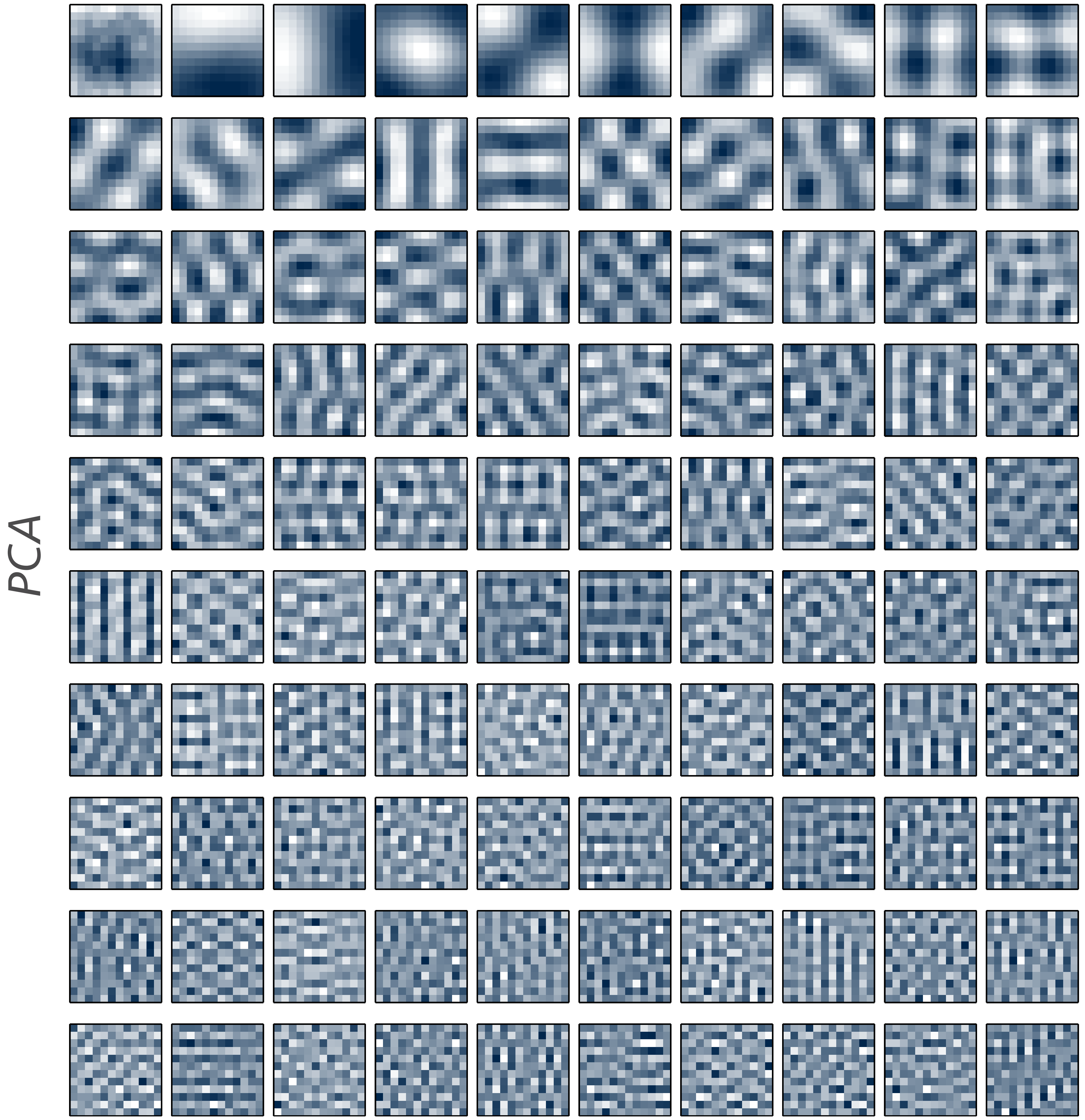
- We know that PCA results in sinusoids

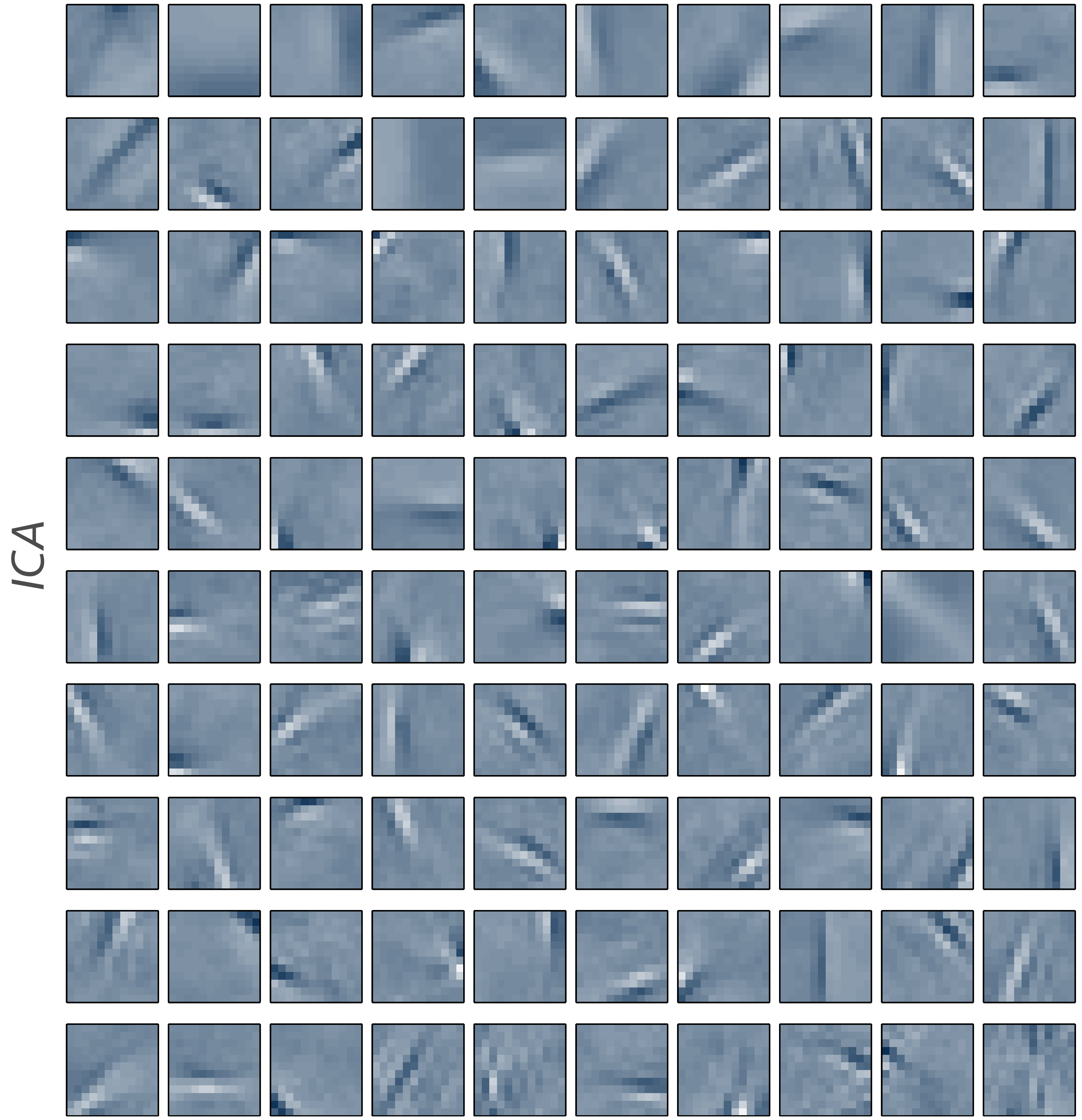
Example features from sounds



Same with images

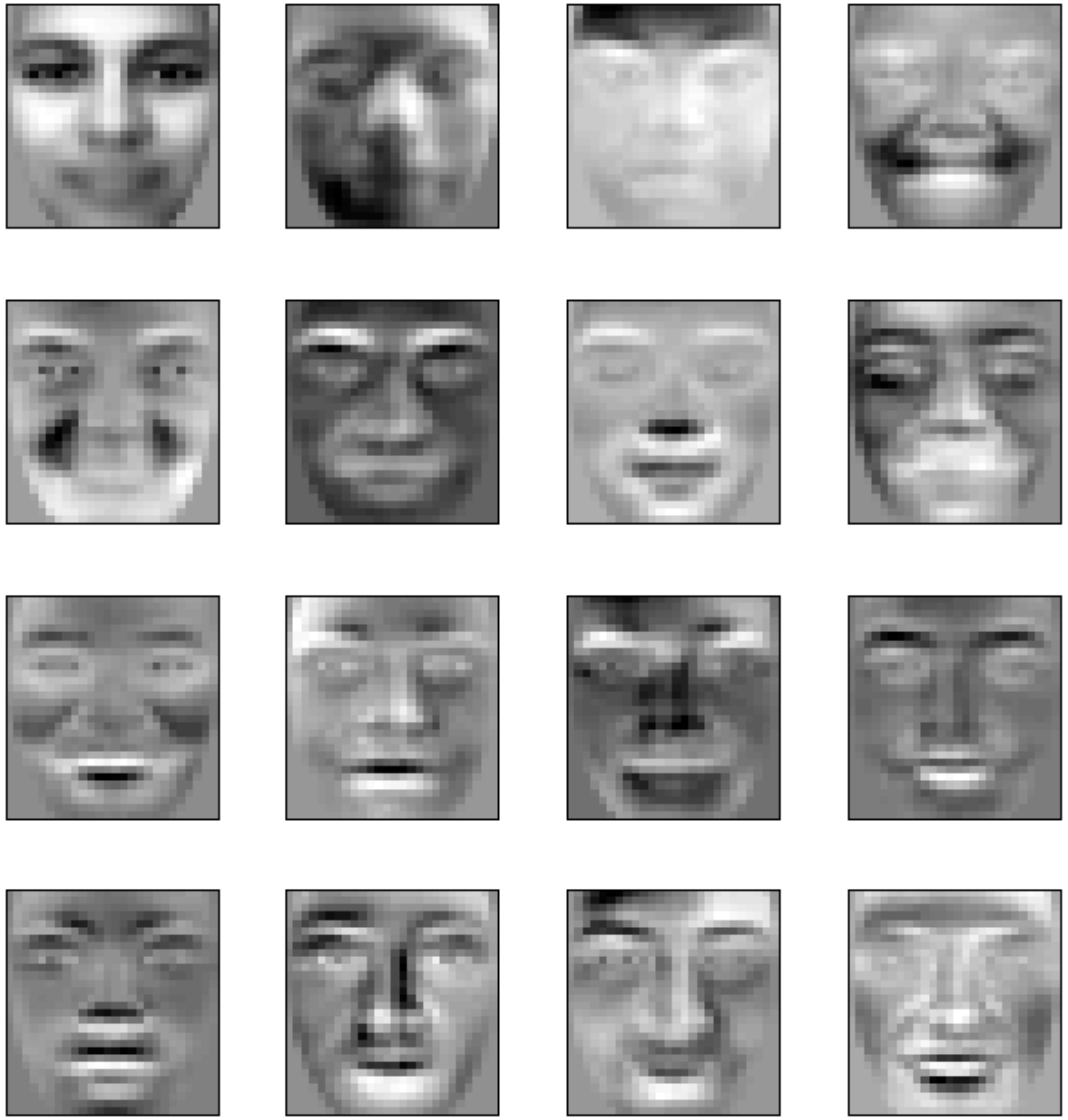
- ICA components look a lot like the V1 receptive fields!



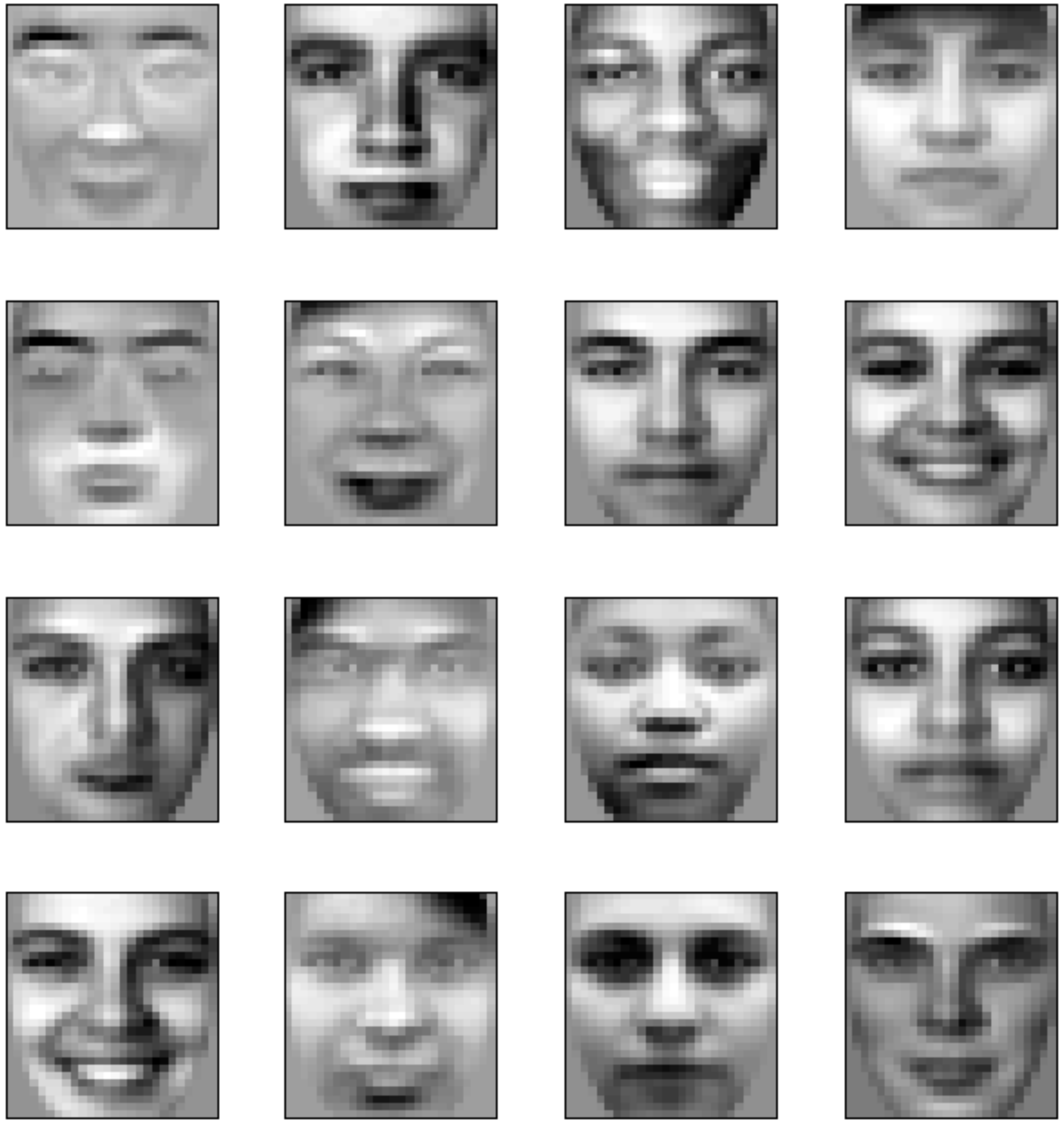


What about faces?

Eigenfaces



ICA-faces



One lesson learned from ICA

- PCA assumes a Gaussian world
  - For a multivariate Gaussian input it does indeed return independent outputs
    - >2nd order Gaussian cumulants are already zero

- ICA work relaxes the Gaussian assumption and assumes a "heavy-tailed" world
  - This is more like the world we live
  - This was a big revelation in machine learning!

Non-Negative Matrix Factorization

- A recent algorithm (Lee & Seung 1999) closely related to components analyses

- Has one magical property
  - It always gives you what you want!

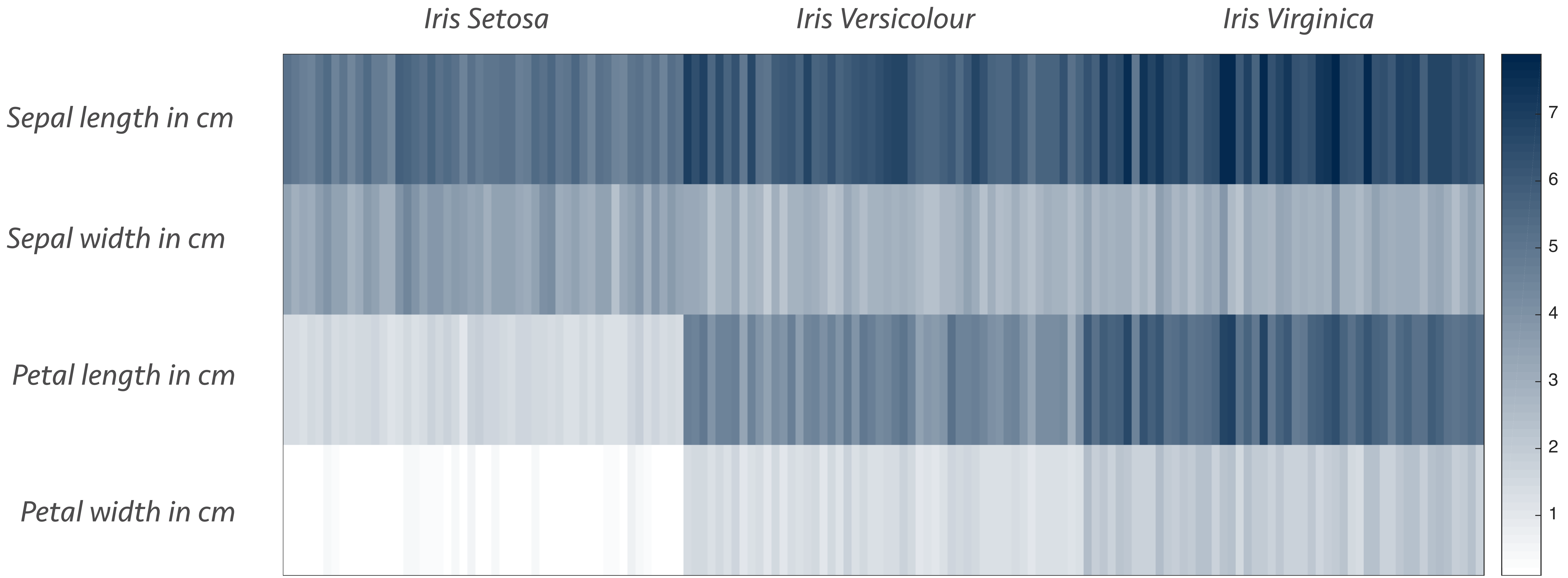
- Has one annoying property
  - Nobody knows quite why!!!

Non-negative data

- We often deal with “non-negative data”
  - Pixels, energies, compositions, counts, etc
- Non-negative data need special treatment
  - Negative valued features can contradict reality

Example case

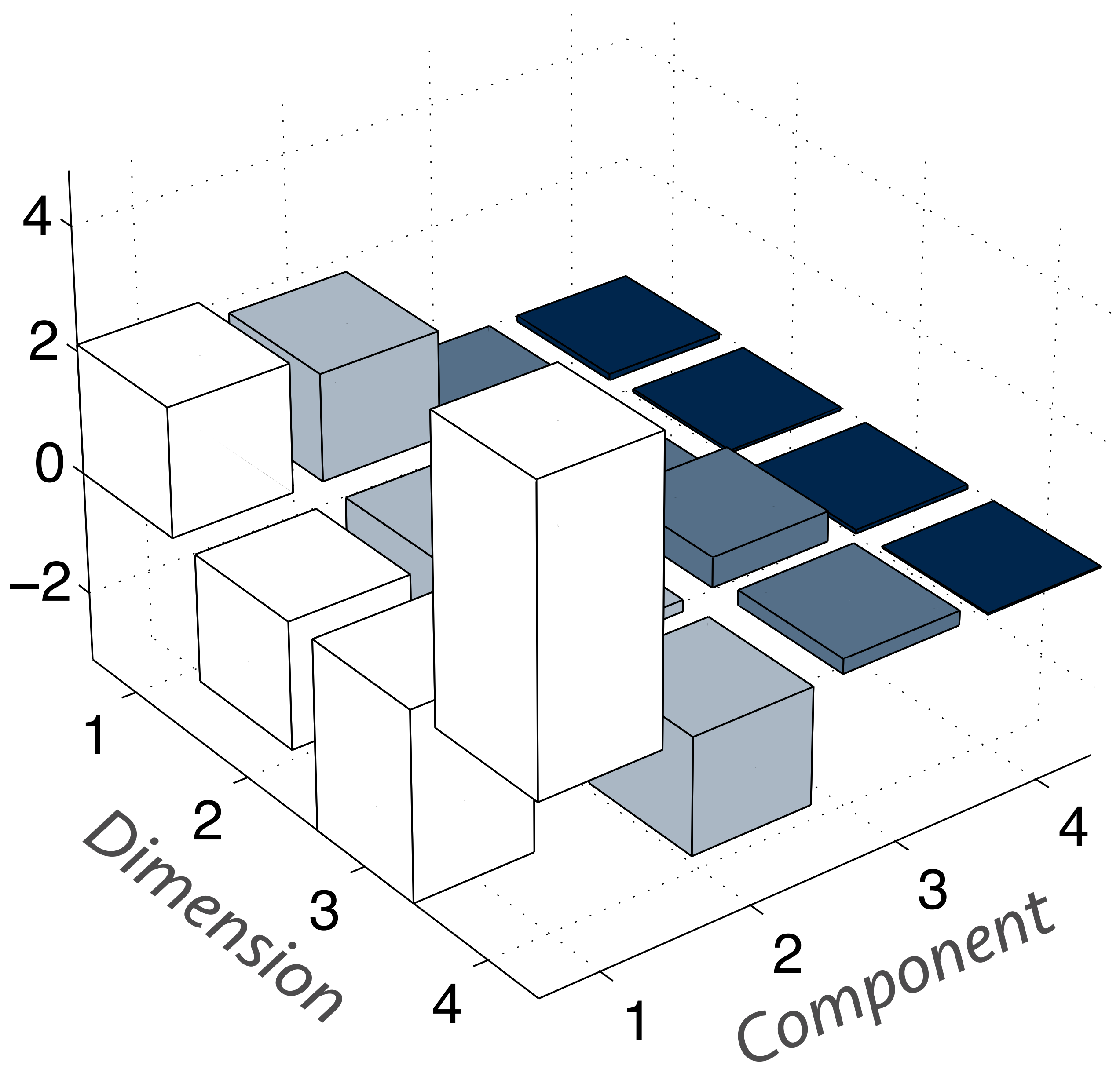
- The Iris data set
  - Each row is a size measurement (i.e. positive)



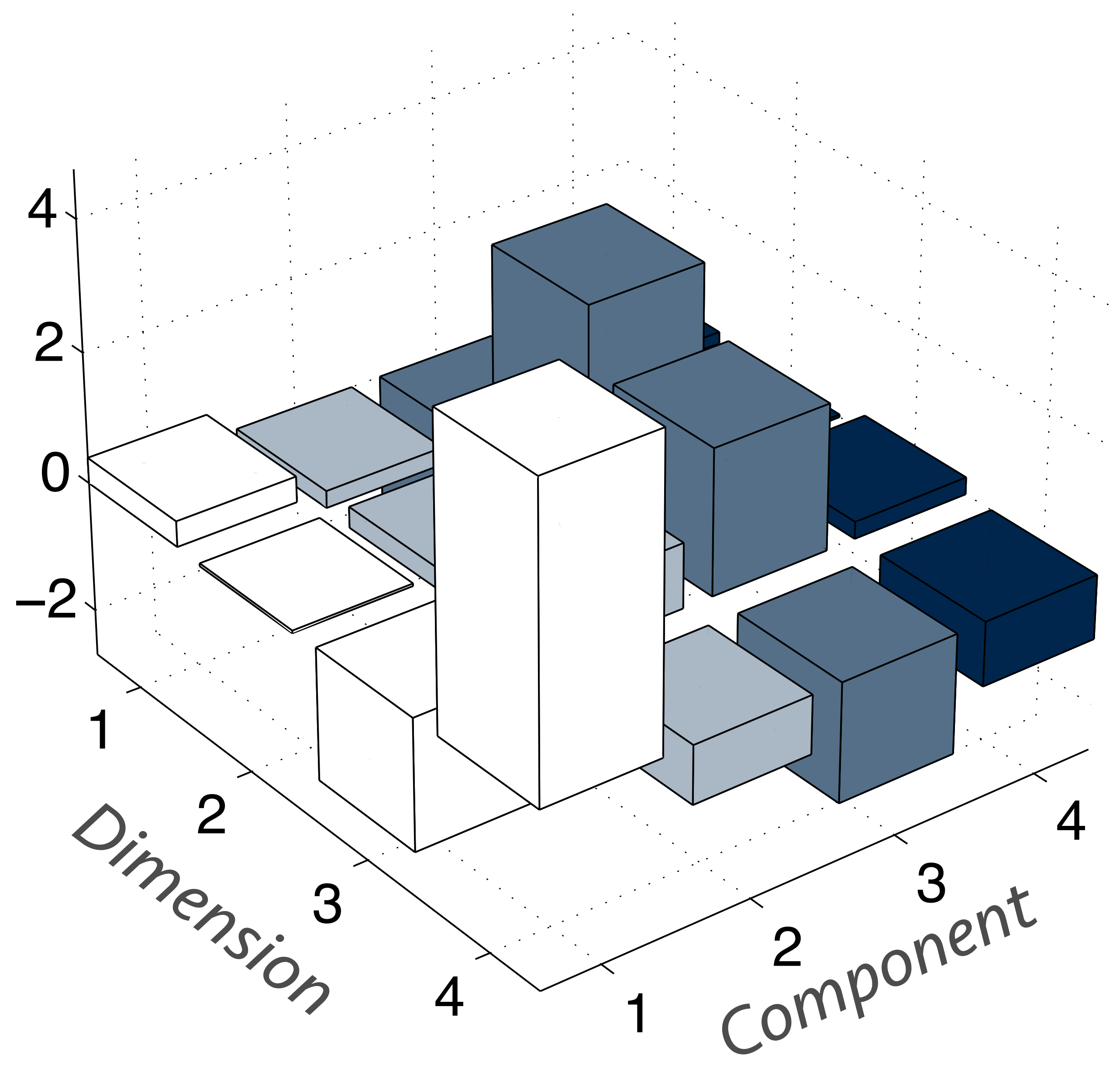
PCA/ICA analysis on iris data

- Both give features that are partly negative
  - What does that mean?

PCA features

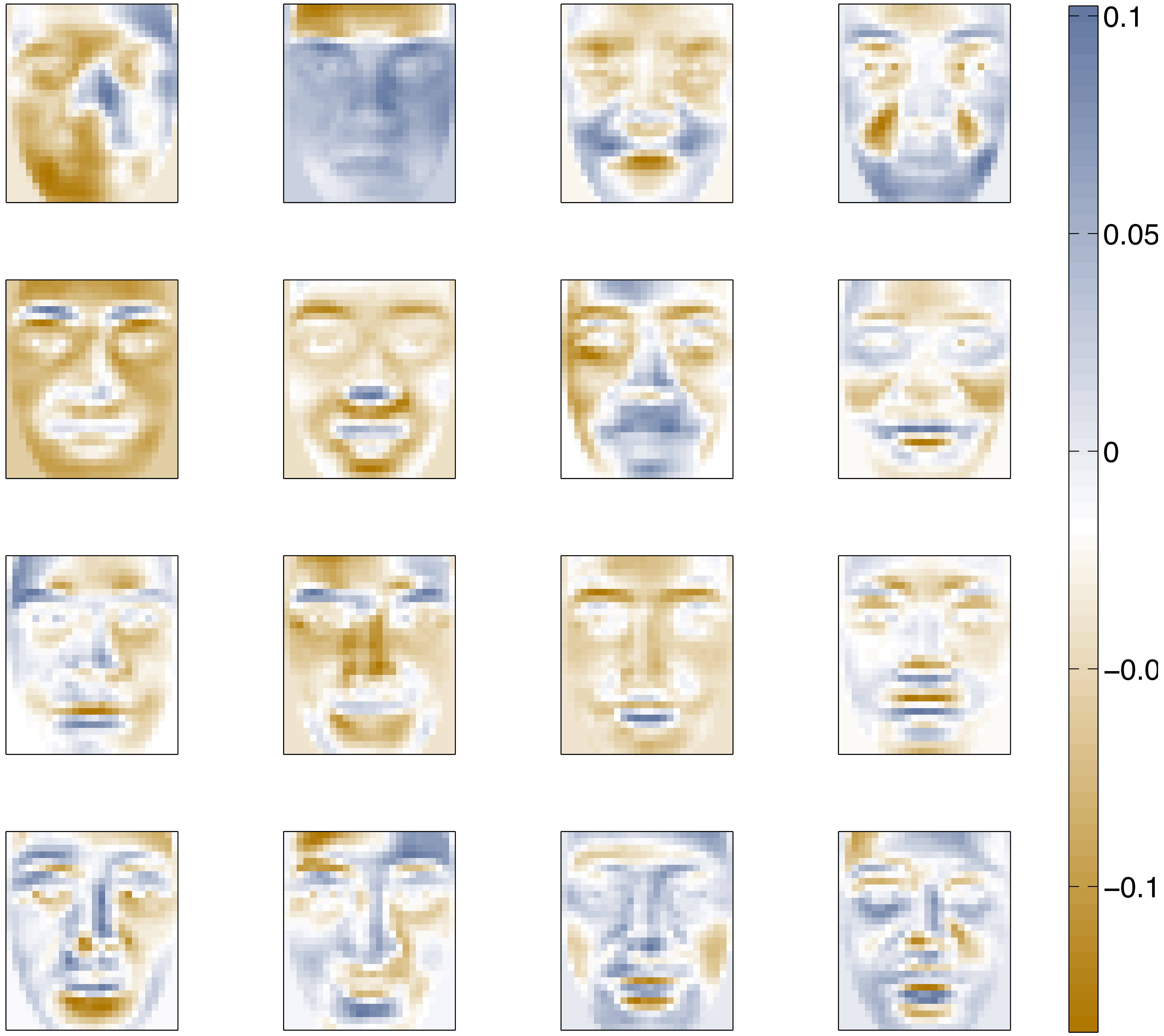


ICA features



Same with eigenfaces

- “Negative” images as bases – why??



Obtaining non-negative features

- Define the factorization problem

$$\mathbf{X} \approx \mathbf{W} \cdot \mathbf{H}$$

$$\mathbf{X} \in \mathbb{R}^{M \times N, \geq 0}, \mathbf{W} \in \mathbb{R}^{M \times R, \geq 0}, \mathbf{H} \in \mathbb{R}^{R \times N, \geq 0}$$

  - This is similar to the PCA/ICA setup
    - R defines the low-rank dimensionality

- How do we solve this one?
  - One known, two unknowns, ugh ...

Solving for the factorization

- We need to estimate two factors
  - Alternate their estimation
- Example algorithm
  - Start with random $\mathbf{W}$
  - estimate an $\mathbf{H}$ given $\mathbf{W}$
  - estimate a new $\mathbf{W}$ given $\mathbf{H}$
  - repeat until convergence

Solving for one factor

- The problem is simpler
  - Only one unknown

$$\min_{\mathbf{W}\ or\ \mathbf{H}} \sum_{i,j} \left| \mathbf{X} - \mathbf{W} \cdot \mathbf{H} \right|^2$$

$$\mathbf{X} \in \mathbb{R}^{M\times N,\geq 0}, \mathbf{W} \in \mathbb{R}^{M\times R,\geq 0}, \mathbf{H} \in \mathbb{R}^{R\times N,\geq 0}$$

- Imposing non-negativity
  - Non-negative least squares (slow)
  - Constrained optimization (slow)
  - Do least-squares and clip the negative numbers (fast!)

A simple NMF algorithm

- Start with random $\mathbf{W}$
  - estimate new $\mathbf{H}$ given $\mathbf{W}$:
    $$\mathbf{H} = \mathbf{W}^{+} \cdot \mathbf{X}$$
    $$\mathbf{H} = \max(\mathbf{H}, 0)$$
  - estimate new $\mathbf{W}$ given $\mathbf{H}$:
    $$\mathbf{W} = \mathbf{X} \cdot \mathbf{H}^{+}$$
    $$\mathbf{W} = \max(\mathbf{W}, 0)$$
  - repeat until convergence

Conceptual problem

- We don't want to use pseudoinverses
  - They imply least-squares minimization
    - Least squares imply Gaussian data
      - We don't have Gaussian data ...
- We define a special distance
  - A variant of KL divergence

$$\min_{\mathbf{W},\mathbf{H}} \left[\sum_{i,j} \mathbf{X}_{i,j} \log \frac{\mathbf{X}_{i,j}}{(\mathbf{W}\cdot\mathbf{H})_{i,j}} - \mathbf{X}_{i,j} + (\mathbf{W}\cdot\mathbf{H})_{i,j} \right]$$

Multiplicative updates

- Using some optimization magic we get:

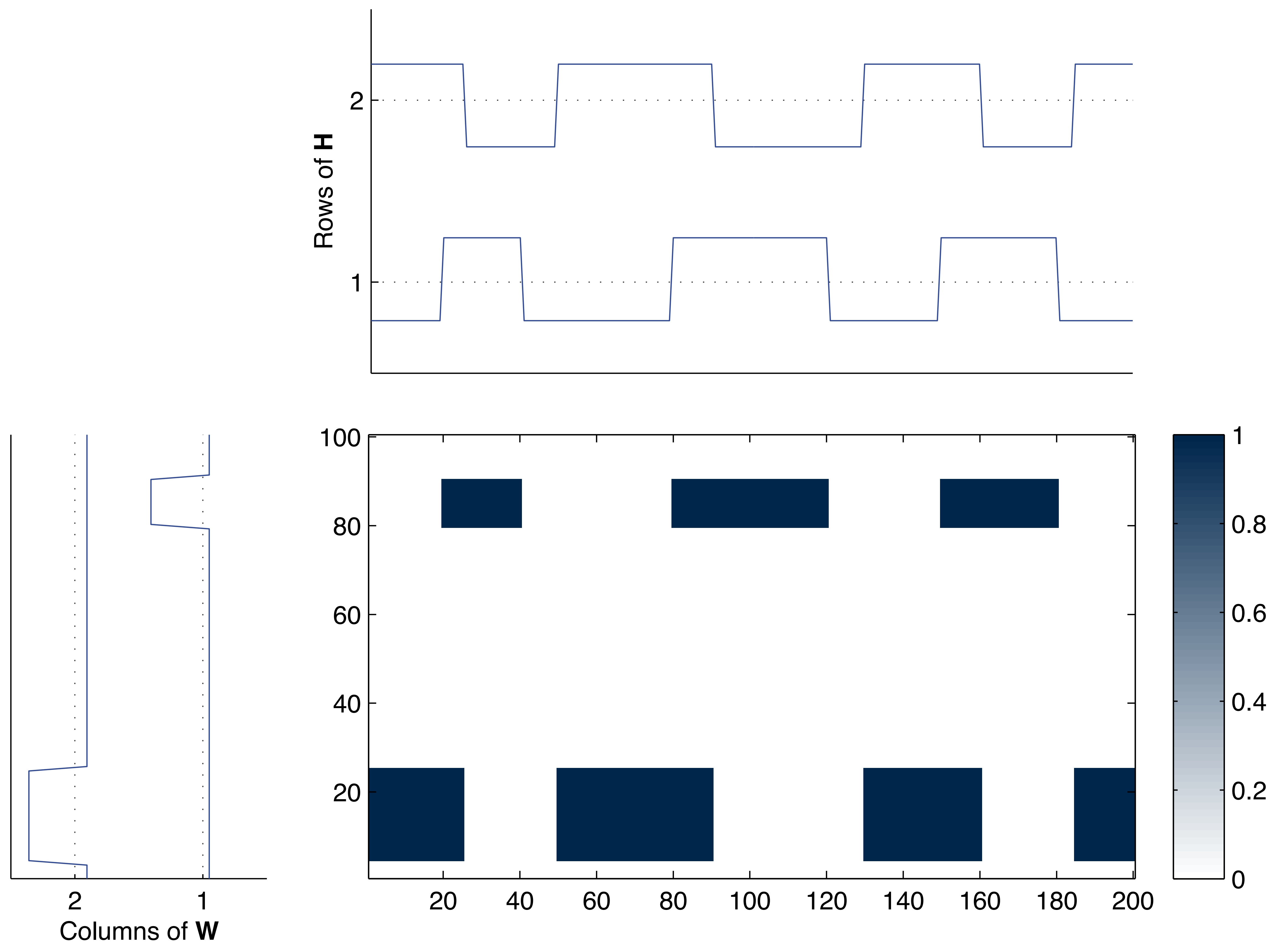
$$\mathbf{W}_{i,j} = \mathbf{W}_{i,j} \sum_k \frac{\mathbf{X}_{i,k}}{(\mathbf{W} \cdot \mathbf{H})_{i,k}} \mathbf{H}_{j,k}$$

$$\mathbf{H}_{j,k} = \mathbf{H}_{j,k} \sum_i \mathbf{W}_{i,j} \frac{\mathbf{X}_{i,k}}{(\mathbf{W} \cdot \mathbf{H})_{i,k}}$$

- Significantly faster operations
  - Just matrix and scalar multiplications
    - No inversions

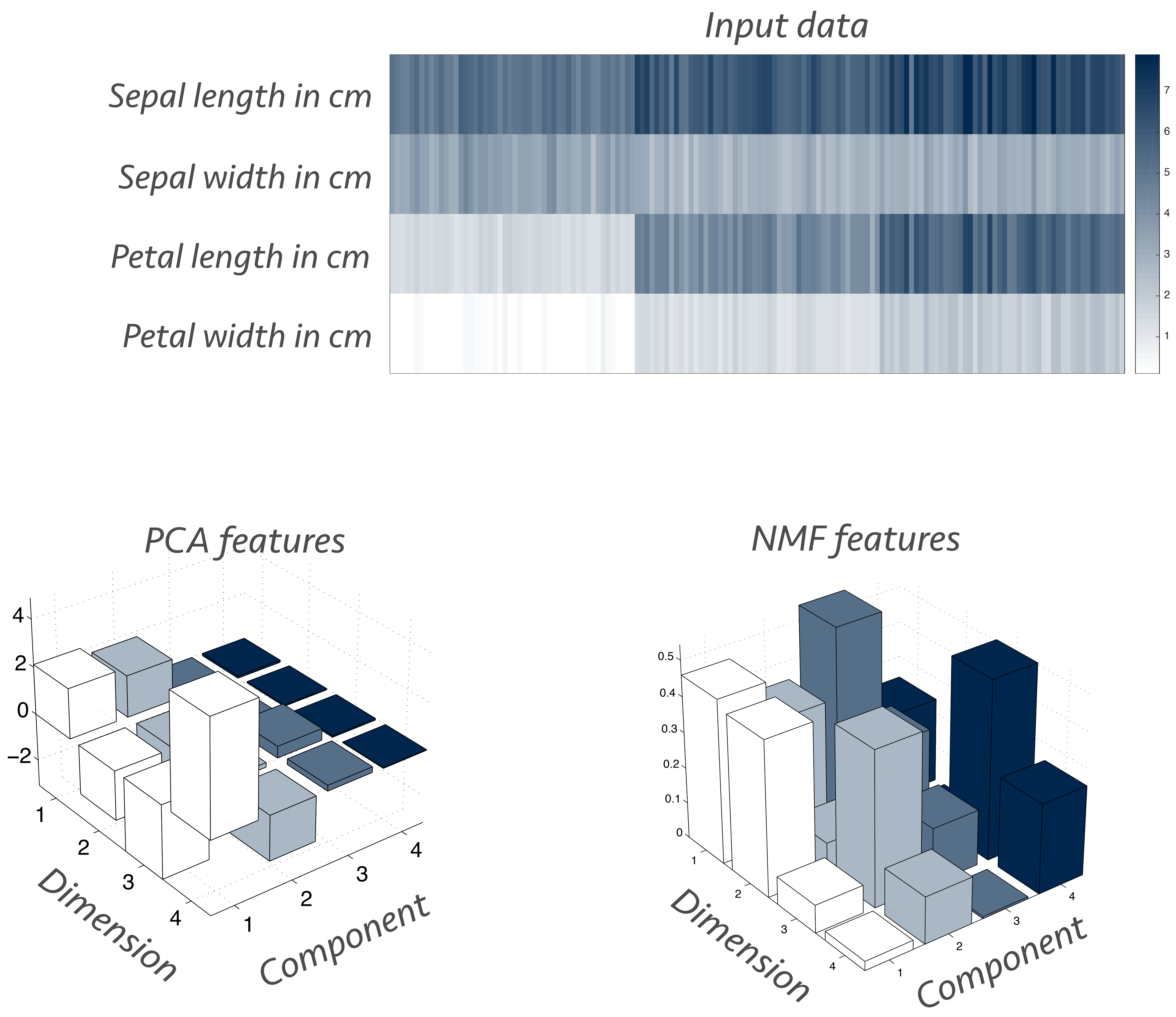
An example

- Start with input $\mathbf{X}$
- NMF will decompose as $\mathbf{X} \approx \mathbf{W} \cdot \mathbf{H}$
- The columns of $\mathbf{W}$ will contain "vertical" information about $\mathbf{X}$
- The rows of $\mathbf{H}$ will contain "horizontal" information about $\mathbf{X}$



Back to the iris data

- NMF on iris provides interpretable results
  - We see the structure
  - The features are meaningful as sizes
- PCA/ICA features
  - Not so useful



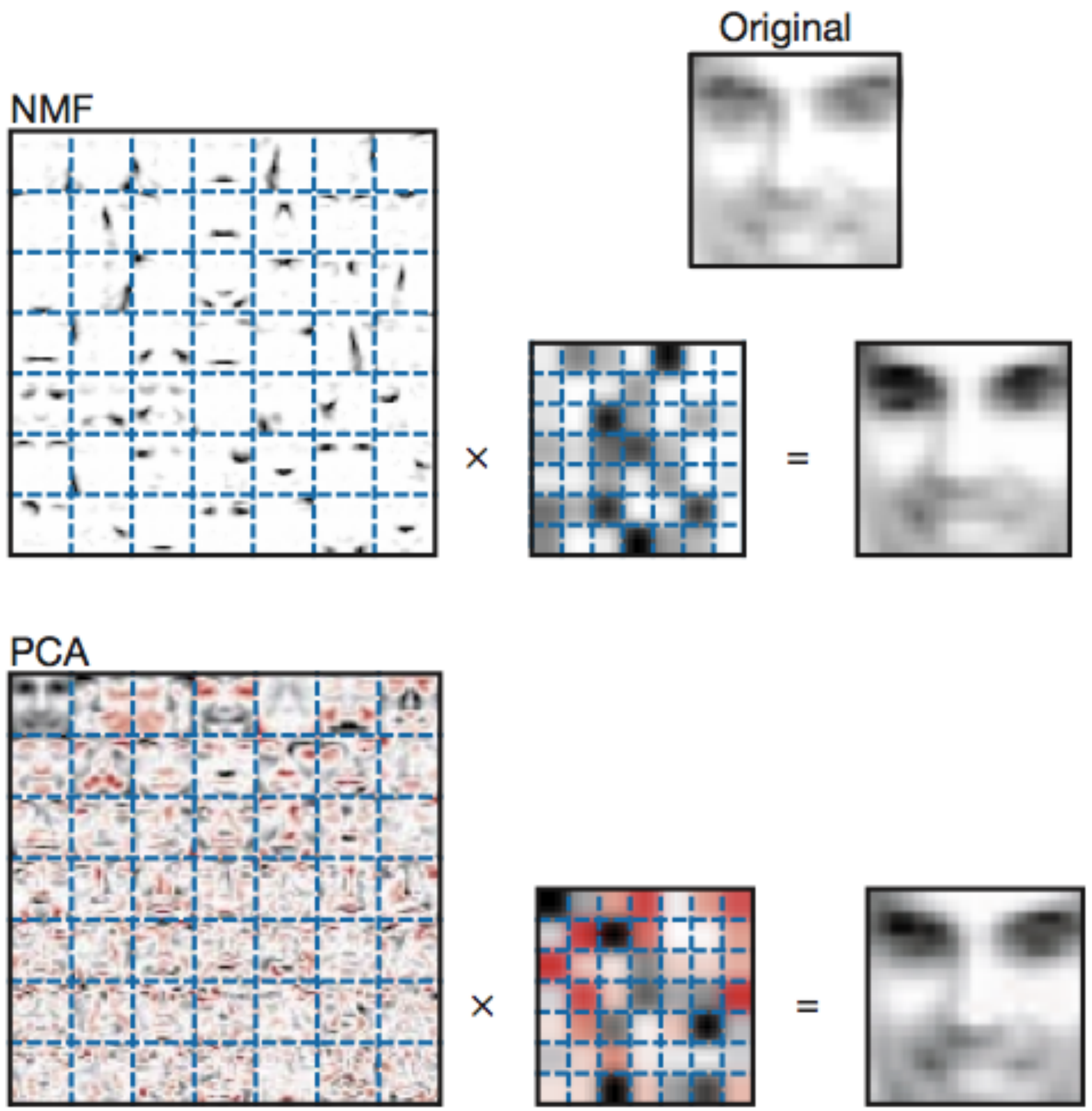
Decomposition by parts

- NMF does "additive decompositions"
  - Explains data in terms of things you add
- This correlates with how we think
  - Scenes are made out of objects
    - We never have "negative" object presence

Example on faces

- Both PCA and NMF describe the data to a good degree
  - Eigenfaces are not interpretable though (very abstract notions)
  - NMF-faces find parts that are additive (noses, eyes, etc.)

- NMF is a better way to explain structured data



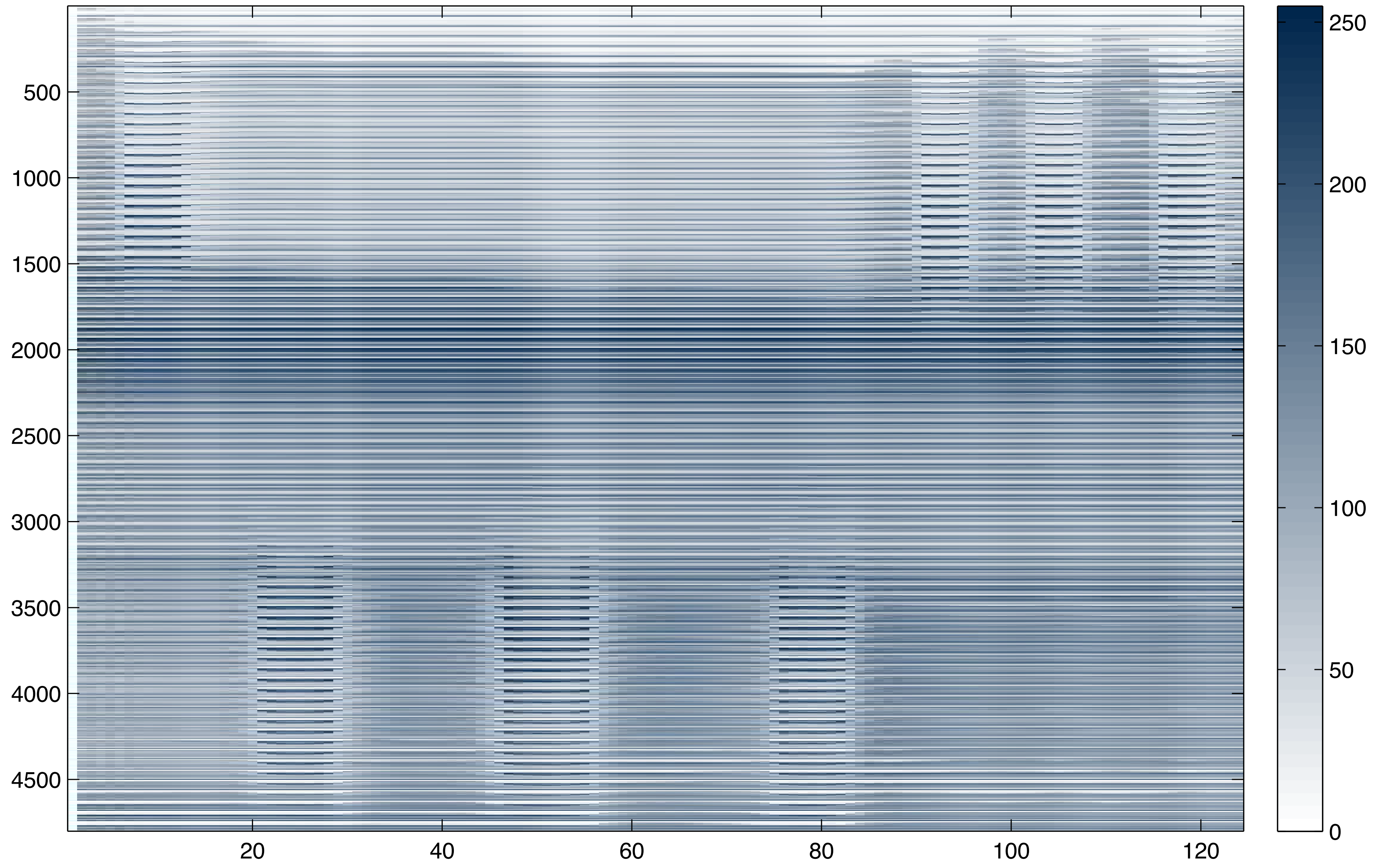
Component analyses on movies

- Movies are fun data for component analyses
  - Immense dimensionality
    - Too much data to train on, we need a more compact form
    - PCA/NMF can do that!
  - Scenes are composed out of elements
    - We want to discover these elements to better analyze the input
    - ICA/NMF can do that!
  - There are visual data and audio data
    - Both exhibit their own structure, often they interrelate
    - All techniques help there!

A Video Example

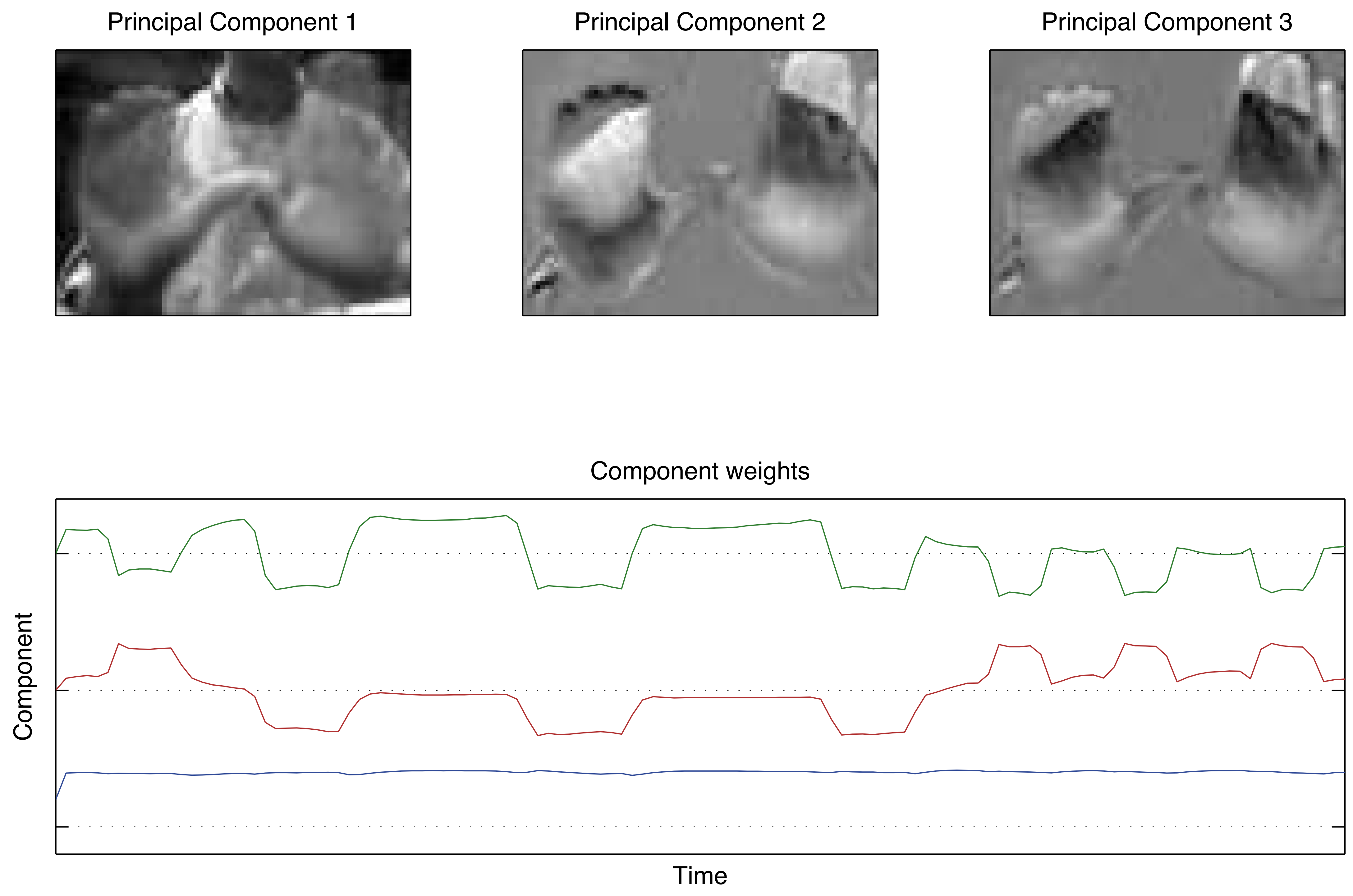
- The movie is a series of frames
  - Each frame is a data point
  - 126, 80 × 60 pixel frames
  - Data will be 4800 × 126

- Using different analyses
  - PCA, ICA, NMF
  - Compare features and weights



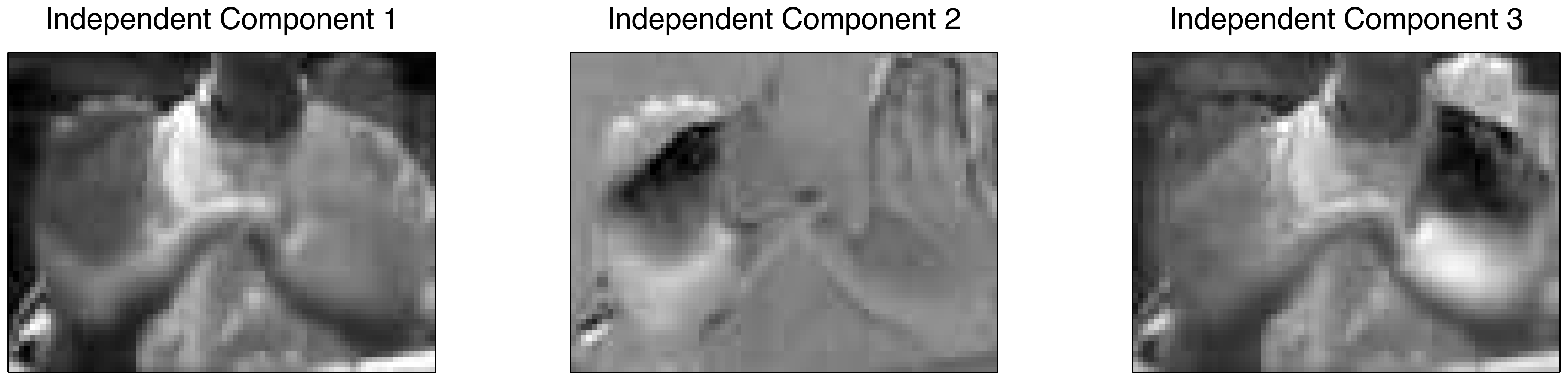
PCA Results

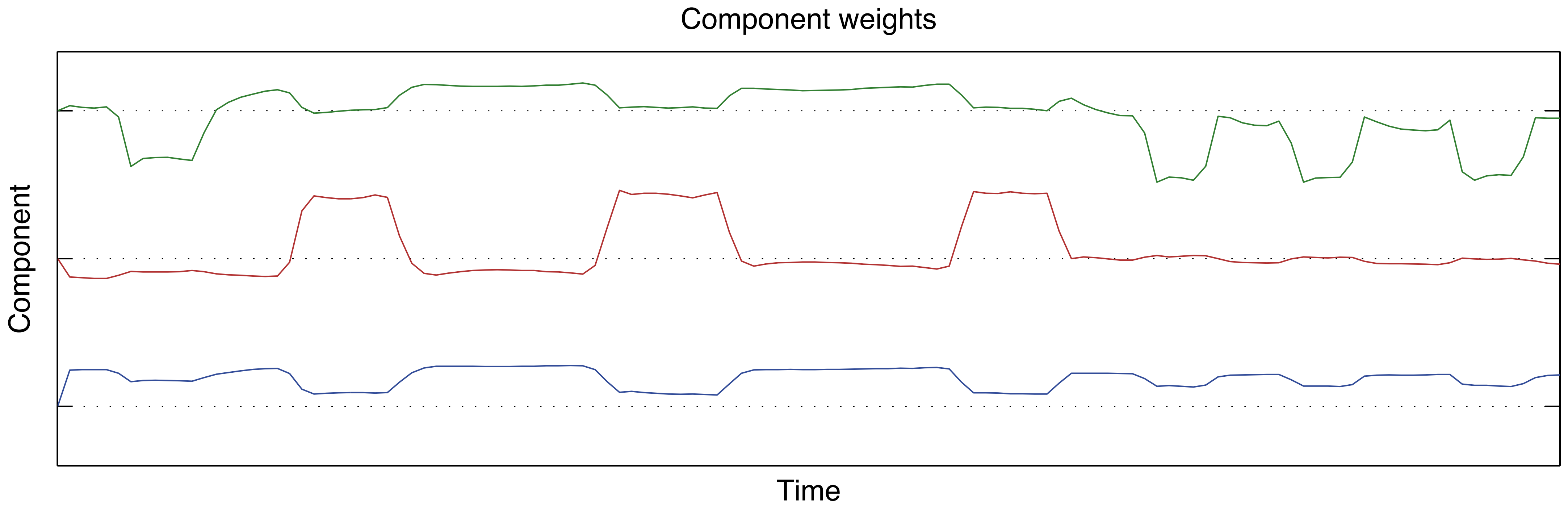
- Nothing special about the visual components
- They are orthogonal pictures
  - Does this mean anything? (not really …)
  - Some segmentation between constant vs. moving parts
- Some highlighting of the action in the weights



ICA Results

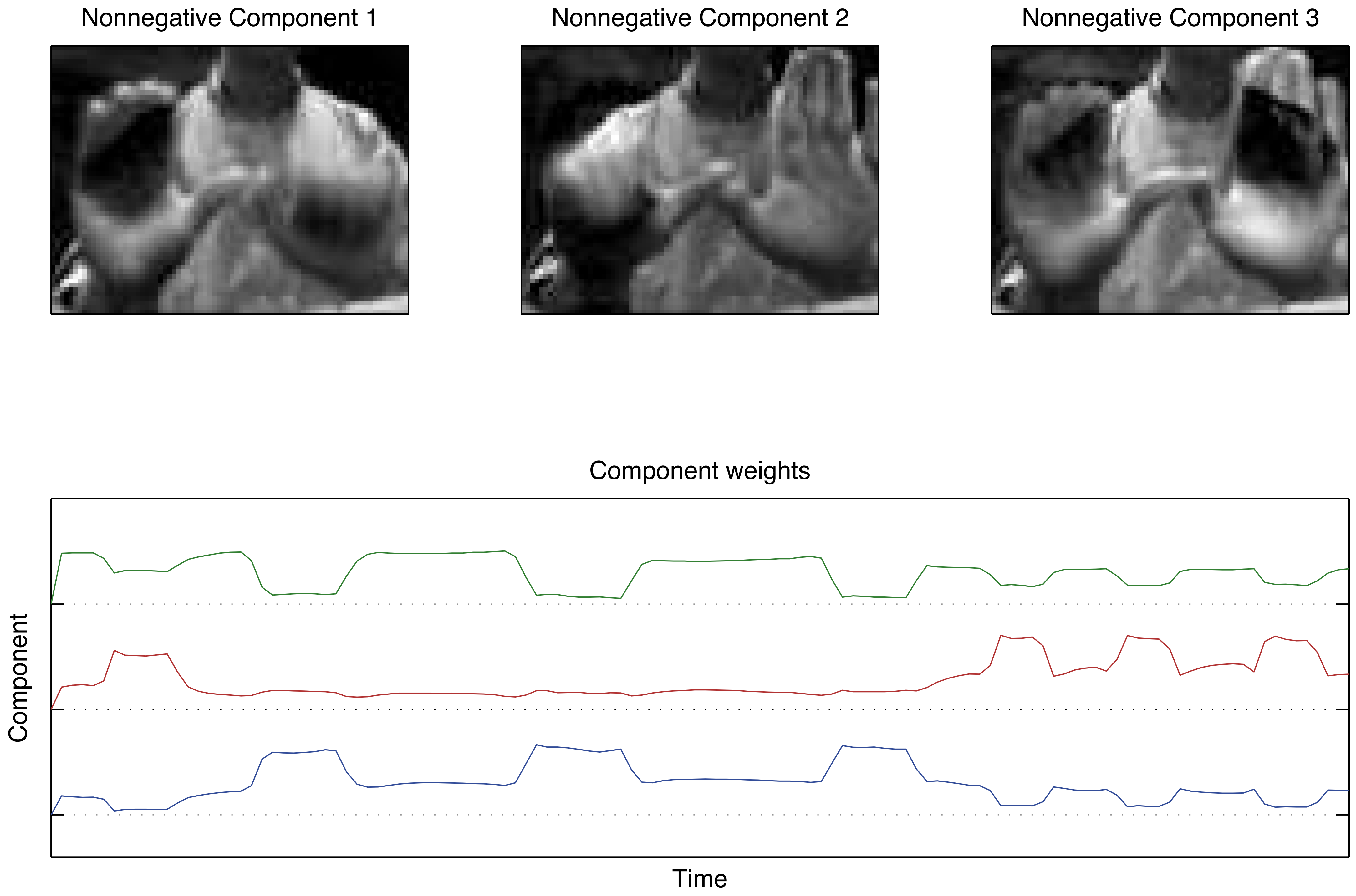
- Much more interesting visual components
- They are independent
  - Unrelated elements (l/r hands, background) are now highlighted
  - We have a decomposition by parts
- Component weights are now describing the scene





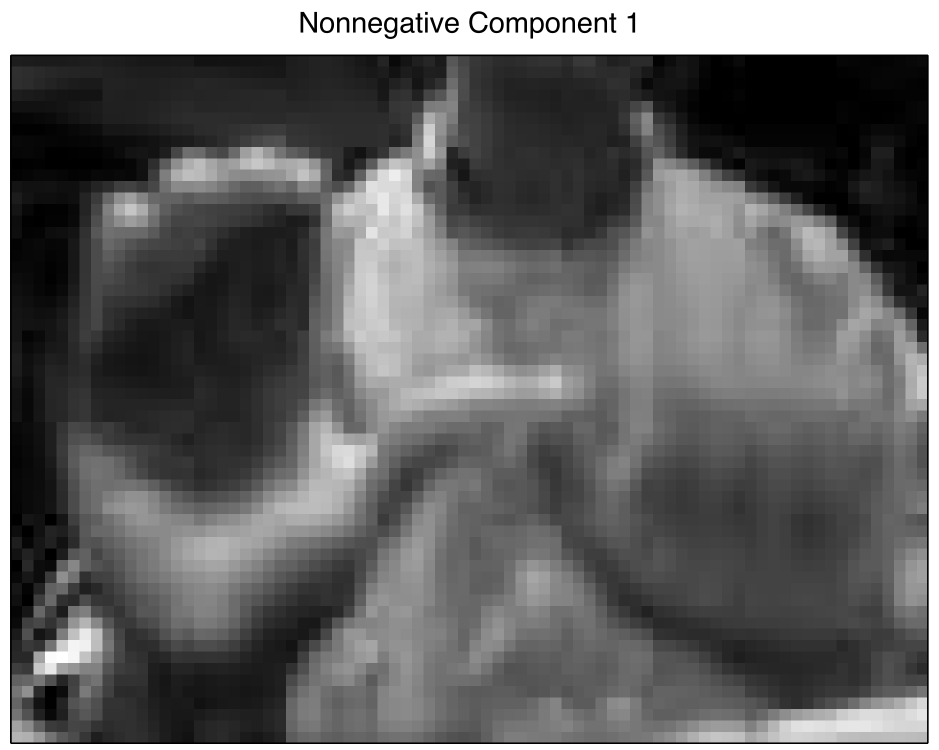
NMF Results

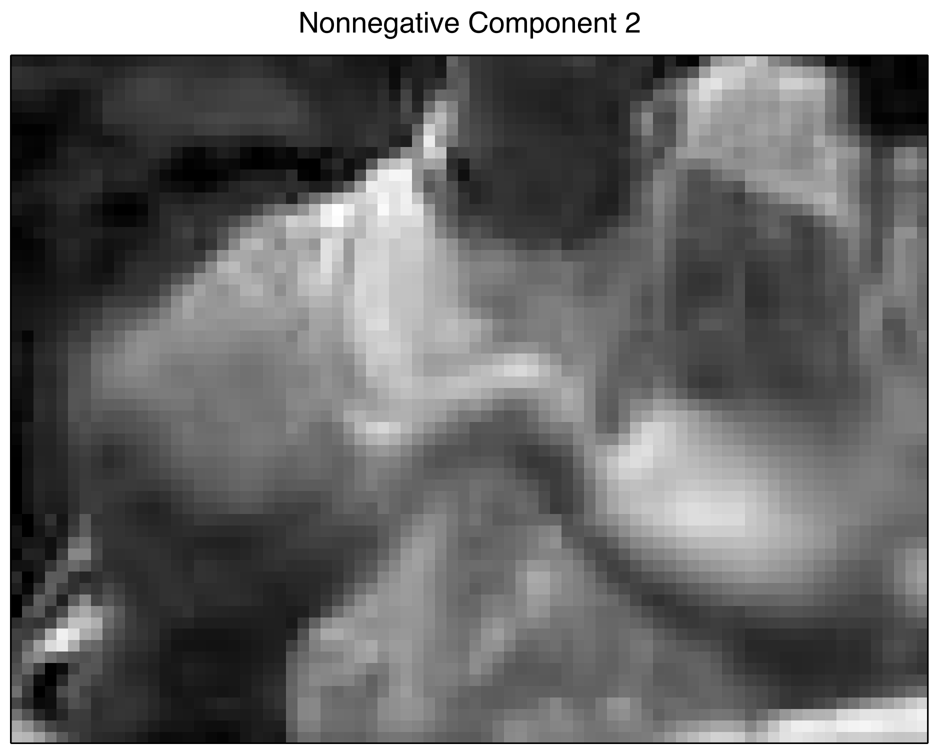
- A different take on the visual components
- We don't know how they relate, but ...
  - They describe the some of the possible states of the video
  - Perhaps a more semantically meaningful representation
- Component weights are as vague as with PCA (because we have more components than we need)

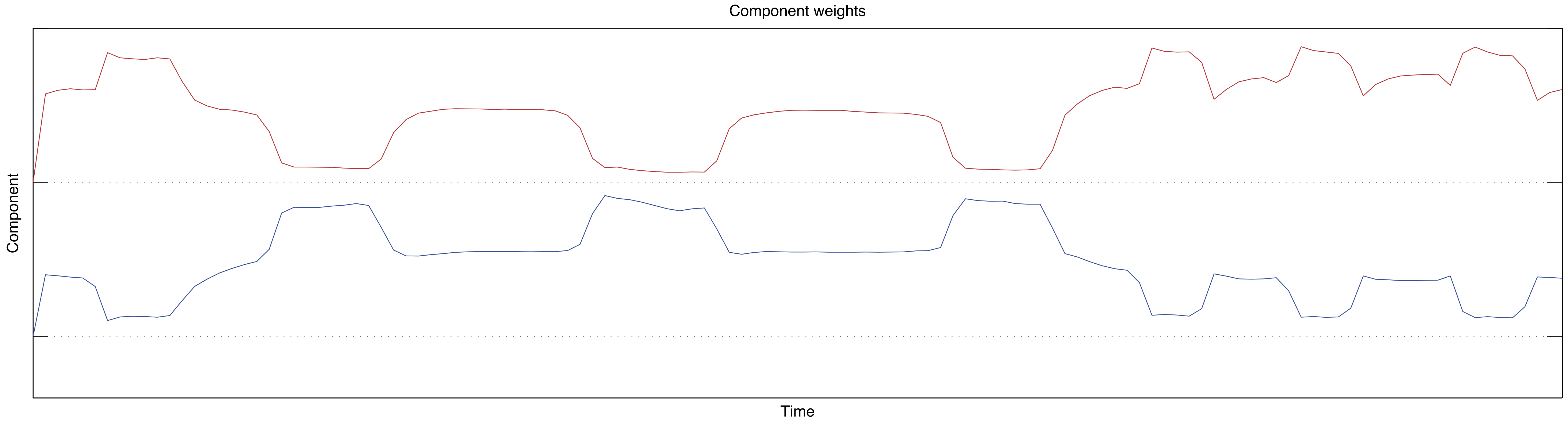


If we use the right dimensions

- The results look exactly as we would want them!





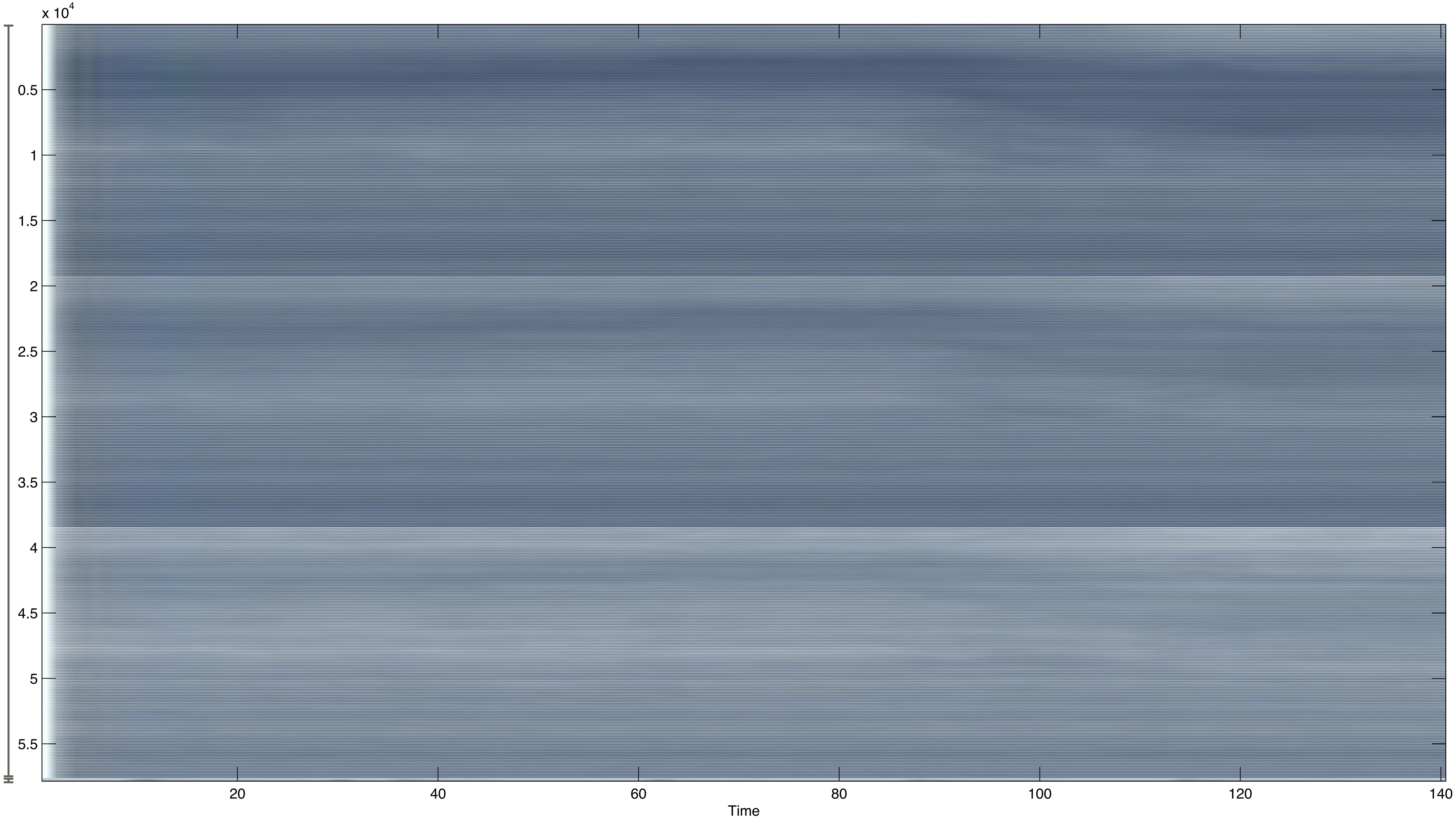


Audio Visual Components?

- We can can even take in both audio and video data and try to find structure
- Sometimes there is a very strong correlation between auditory and visual elements
- We should be able to discover that automatically

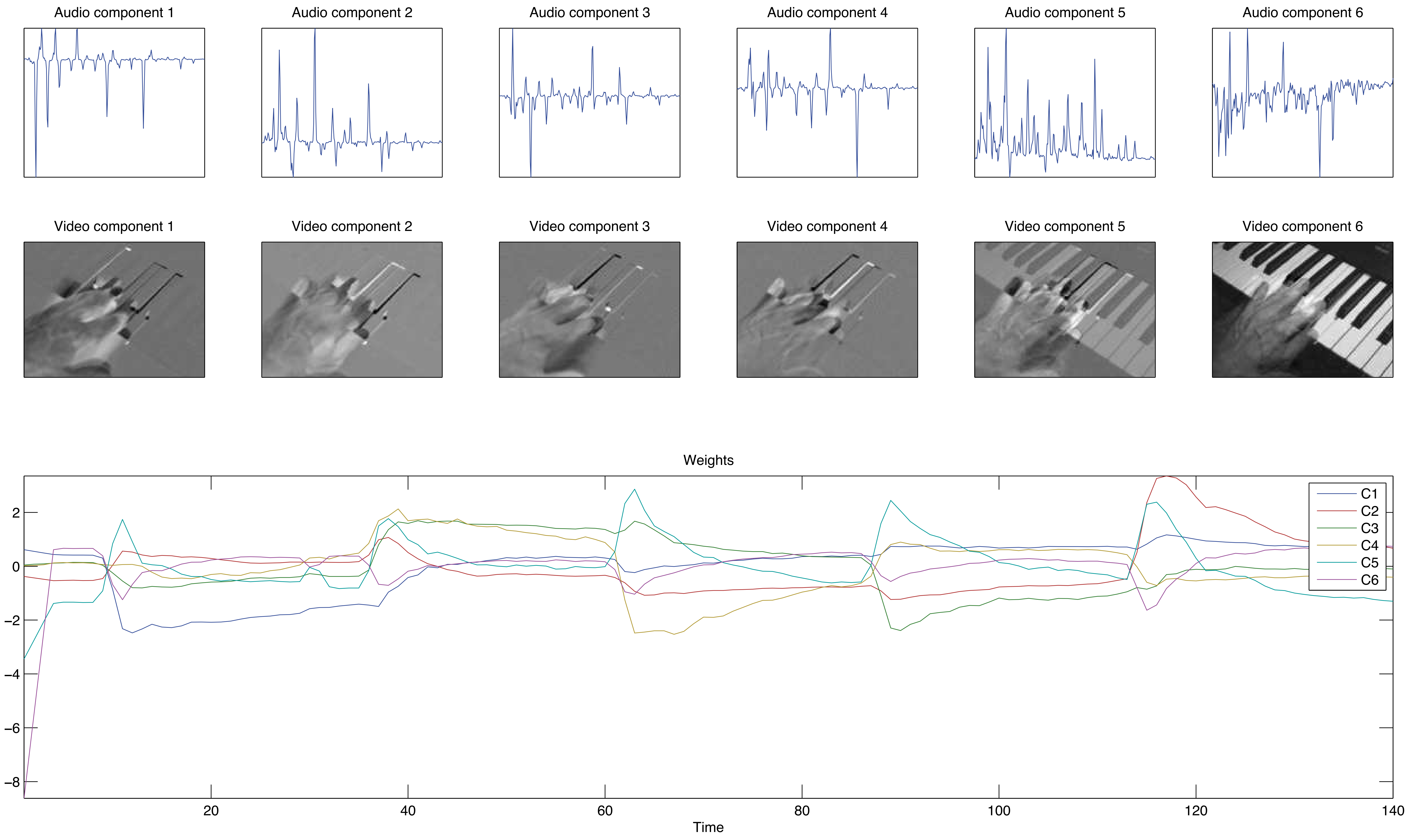
What does the data look like?

57,600 pixel dimensions

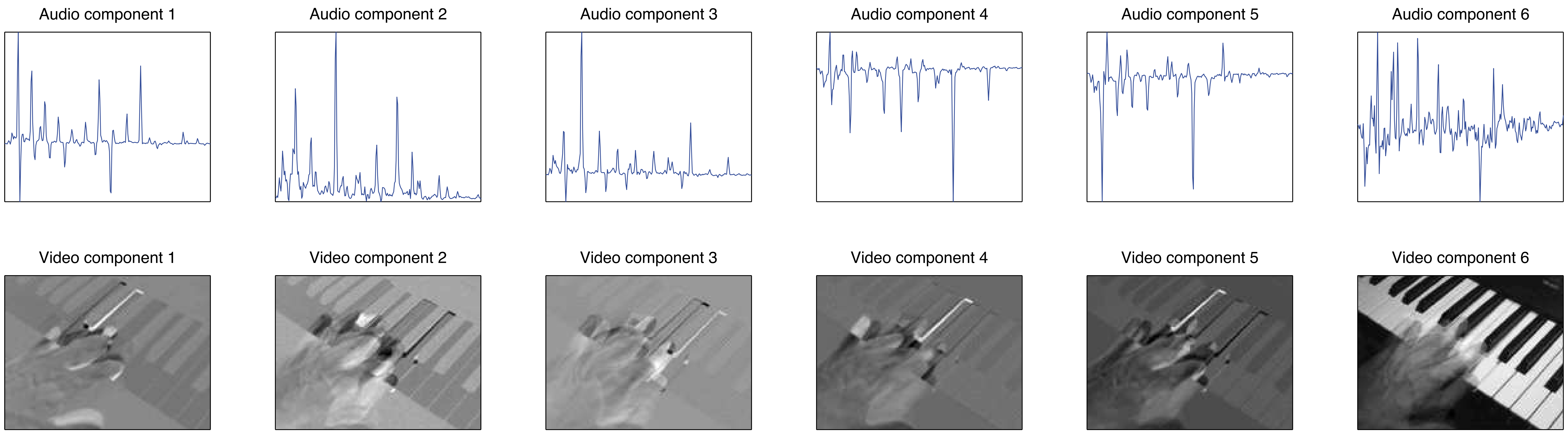


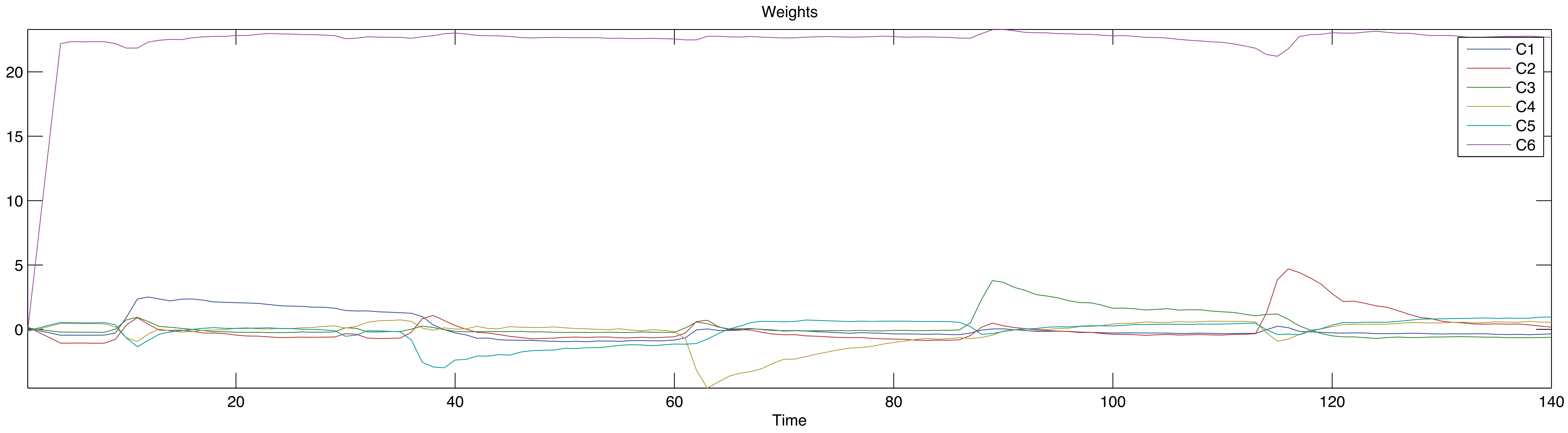
257 audio dimensions

Audio/Visual PCA components

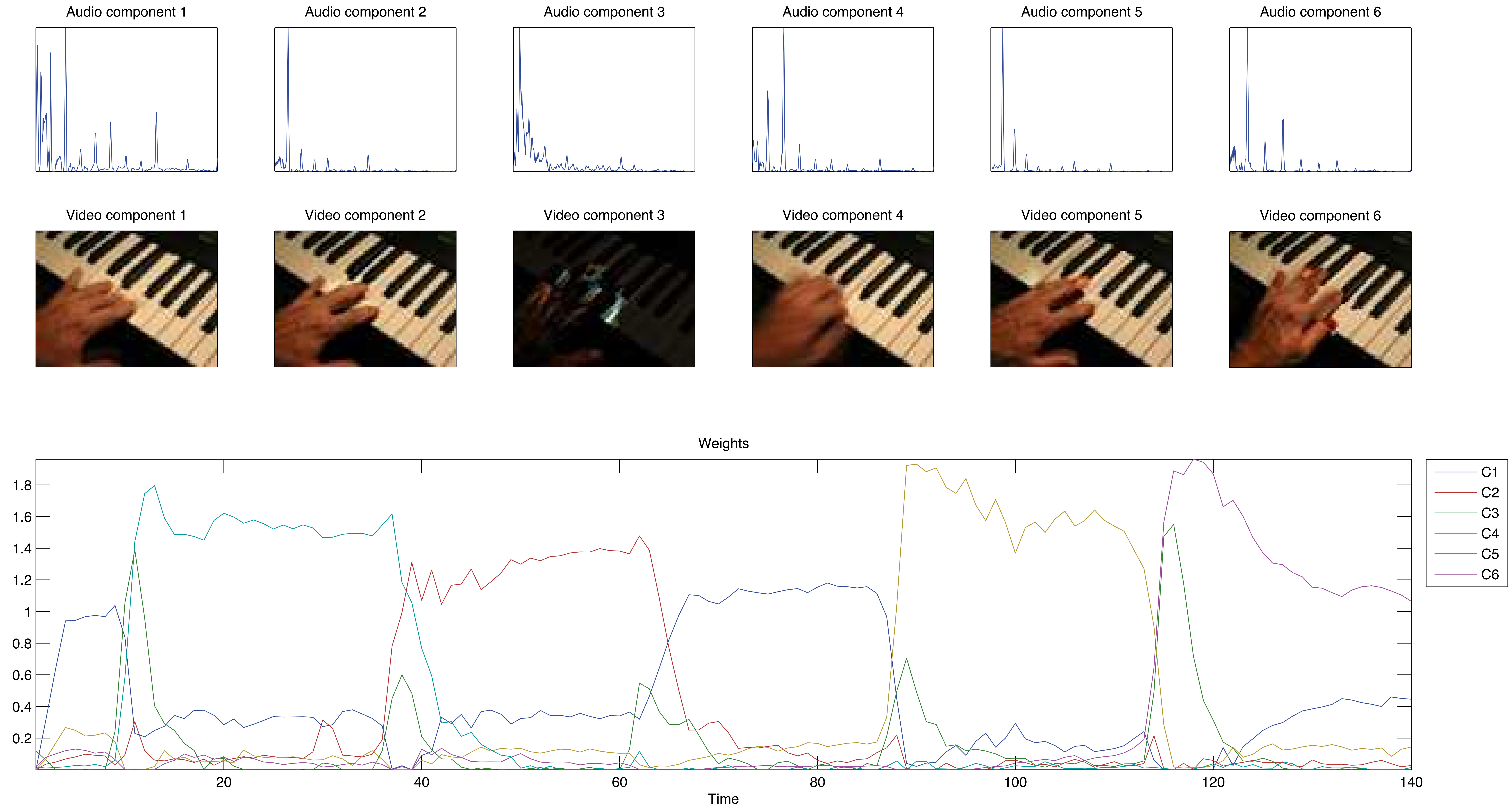


Audio/Visual ICA components

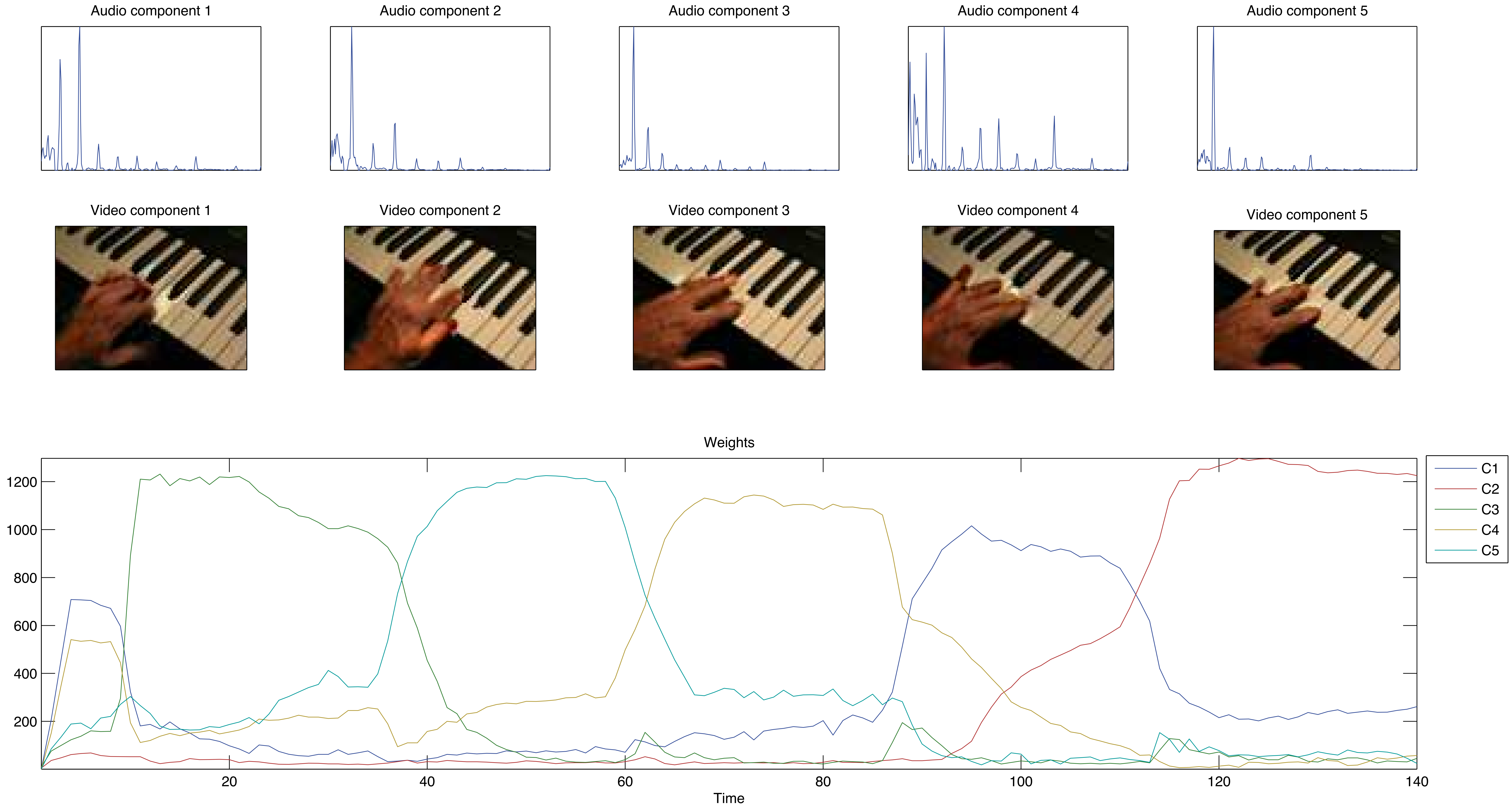




Audio/Visual NMF components



Audio/Visual NMF components



PCA, ICA or NMF?

- Depends on what you want to do
  - PCA does a fantastic job in dimensionality reduction
  - ICA provides a clean output
    - And is perceptually more relevant
  - NMF provides interpretable outputs
    - But only for non-negative data
- As usual there is no right answer
  - When in doubt try them all!

Recap

- Independent Component Analysis
  - Obtains maximal independence
  - Does not reduce dimensionality
- Non-Negative Matrix Factorization
  - Best for analysis of non-negative data
    - pixels, energies, count data, etc ...
  - No particular statistical property though

Next lecture

- Last on features for a while
- Non-linear methods
  - What do do when your data looks really strange
- Manifolds and embedding
  - Finding latent structure in high dimensions

Reading

- Textbook sections 6.5-6.6
- Independent Component Analysis (optional)
  - http://www.cis.hut.fi/aapo/papers/IJCNN99_tutorialweb/
- Natural stimuli statistics (optional)
  - http://redwood.berkeley.edu/bruno/papers/nature-paper.pdf
  - ftp://ftp.cnl.salk.edu/pub/tony/vis3.ps.Z
  - http://www.cnbc.cmu.edu/cplab/papers/Lewicki-NatNeurosci-02.pdf
- Non-negative Matrix Factorization (optional)
  - http://hebb.mit.edu/people/seung/papers/ls-lponm-99.pdf